Strategies to measure a quantum state

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Abstract

We consider the problem of determining the mixed quantum state of a large but finite number of identically prepared quantum systems from data obtained in a sequence of ideal (von Neumann) measurements, each performed on an individual copy of the system. In contrast to previous approaches, we do not average over the possible unknown states but work out a “typical” probability distribution on the set of states, as implied by the experimental data. As a consequence, any measure of knowledge about the unknown state and thus any notion of “best strategy” (i.e. the choice of observables to be measured, and the number of times they are measured) depend on the unknown state. By learning from previously obtained data, the experimenter re-adjusts the observable to be measured in the next step, eventually approaching an optimal strategy.

We consider two measures of knowledge and exhibit all “best” strategies for the case of a two-dimensional Hilbert space. Finally, we discuss some features of the problem in higher dimensions and in the infinite dimensional case.

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1 Introduction

The topic of this paper is the problem of determining a quantum state from measurement data. We consider a quantum system described by a Hilbert space $\mathcal{H}$ of (finite) dimension $d$. Given a large but finite number of copies of the system, all prepared in the same quantum state $\tau$, we shall be allowed to perform an arbitrary (ideal) measurement in each copy. What knowledge about the state $\tau$ do we have after these measurements, and what is the best strategy to maximize the information gained? Several authors have considered problems of this type. Their approaches differ in some respects, in particular regarding the measurement strategy and the way how the knowledge about the unknown state $\tau$ is quantified.

The strategy analyzed by Wootters and Fields [1] consists of choosing – once and for all – a family of $d+1$ observables, and measuring each one in a separate copy of the system an equal number of times. The knowledge gained in these measurements is quantified in terms of the average (over all possible unknown states) of an appropriately defined “uncertainty volume” in the set of states (which essentially stems from the Shannon [2] information measure). They arrive at the result that the average gain of knowledge in such a procedure is maximal if the $d+1$ observables measured are mutually unbiased (complementary). This optimal strategy is, by definition, independent of the actual (unknown) state $\tau$. Their paper is sometimes referred to as proving that the use of mutually unbiased observables is the most efficient determination of an unknown quantum state by means of successive measurements.

Peres and Wootters [3] conjectured that an appropriately designed single combined measurement on a number of identically prepared copies of a quantum system is more efficient than a sequence of measurements on the individual systems (a sequential measurement). Moreover, they provided evidence that generalized (POVM based, see Refs. [4][5][6]) measurements are more effective than ideal measurements of the von Neumann type [7]. Their measure of knowledge is based on the Shannon information measure as well.

In a special scenario, Massar and Popescu [8] showed that a combined measurement is more efficient than a sequential one, thus proving (“not in its letter, but in its spirit”) Peres and Wootters’ conjecture. In their work, knowledge is measured by a “score” function defined as the average (over all possible unknown states) of an
expression quantifying the difference between a candidate state and the unknown one.

In apparent contradiction to these results, Brody and Meister [9] showed that the minimum Bayesian decision cost – taking properly into account what is known \( \text{\textit{\`a priori}} \) about the unknown state – is the same for sequential as for combined measurements. They pointed out that the optimal strategy in determining a quantum state depends on the details of the approach, in particular on how the \( \text{\textit{\`a priori}} \) knowledge is treated.

In order to help clarifying these issues, we present a further approach to the state determination problem. Thereby, we focus on the original scenario of a sequence of ideal (von Neumann) measurements on individual copies of the system. We first compute a “typical” probability distribution on the set \( S \) of states achieved after a (large) number of measurements, thereby \textit{retaining the dependence on the unknown state} \( \tau \) throughout the analysis. In other words: we will \textit{not} perform an average over all possible unknown states. Thus, any measure of knowledge (of which we discuss two variants, one being related to the “uncertainty volume” as considered by Wootters and Fields) depends on \( \tau \), and so do the “best strategies”. After having arrived at (two variants of) a general variational principle determining what is a best strategy, we solve the problem of finding these strategies in very detail in two dimensions \((d = 2)\), and discuss some features of the problem in higher dimensions.

In contrast to the scenario considered by Wootters and Fields, our experimentalist learns from previously obtained data and uses them to re-adjust the observable measured in the next step, eventually approaching the best strategy for the unknown state \( \tau \). We show that, in dimensions larger than 2, the best strategy is sometimes \textit{not} provided by a family of mutually unbiased observables.

We conclude the paper by giving some remarks on the infinite dimensional case.
2 Derivation of the probability density

Let us begin introducing some notation. The spectral decomposition of any observable (hermitean linear operator) reads

\[ A = \sum_{a \in \text{Sp}(A)} a P_a, \]  

(2.1)

where \( \text{Sp}(A) \) denotes the spectrum (set of eigenvalues) of \( A \), and \( P_a \) are the (unique) hermitean projections onto the respective eigenspaces (the spectral projections) satisfying \( P_a P_b = 0 \) for \( a \neq b \), and summing up to the identity operator: \( \sum_{a \in \text{Sp}(A)} P_a = 1 \). In a given state (density matrix) \( \rho \), the probability to obtain the outcome \( a \in \text{Sp}(A) \) in a measurement of \( A \) is given by

\[ w_a(\rho, A) = \langle P_a \rangle_\rho \equiv \text{Tr}(\rho P_a), \]  

(2.2)

the symbol \( \langle \rangle_\rho \) denoting the expectation value in the state \( \rho \).

Now suppose we are given \( n \) copies of a quantum system, prepared to be in the same – unknown – quantum state \( \tau \), and we are allowed to perform a sequence of measurements of \( n \) observables \( (A_1, A_2, \ldots, A_n) \), each on one copy of the system. This setting guarantees that the outcomes, collectively denoted as

\[ \Lambda \equiv (a_1, a_2, \ldots, a_n), \]  

(2.3)

are statistically independent of each other. Given these data – what can we say about the state? This is a case for an application of Bayes’ Theorem of elementary probability theory: Given a domain \( D \) in the space \( S \) of states, we ask for a probability that the measurement outcomes \( \Lambda \) arise from a state contained in \( D \). In other words, we ask for a probability distribution describing the likelihood of \( \rho \) to be responsible for the experimental data. This requires the assumption of an \( \text{à priori} \) likelihood, i.e. a probability measure on \( S \). A natural candidate is the measure \( D\rho \) induced by the Hilbert-Schmidt geometry – see (2.21) below –, but in order to be open for different choices, we include an additional density \( \mu(\rho) \). We will see that things do not depend heavily on this quantity. Whatever choice is made, Bayes’ Theorem tells us that the desired probability distribution on the space of states is given by

\[ p_\Lambda(\rho) = C \mu(\rho) \prod_{j=1}^{n} w_{a_j}(\rho, A_j) \equiv C \mu(\rho) \exp \left( \sum_{j=1}^{n} \ln w_{a_j}(\rho, A_j) \right), \]  

(2.4)
where the constant $C$ is chosen such that

$$\int_S \mathcal{D}\rho \, p_\Lambda(\rho) = 1. \quad (2.5)$$

This is the starting point for our analysis.

The probability density (2.4) is defined for any experimental record $\Lambda$ consisting of all measurement outcomes (2.3). For small $n$, the statistical fluctuations in the data lead to a strong dependence of $p_\Lambda(\rho)$ on $\Lambda$. When the number of measurements is increased in an appropriate way, the fluctuations get suppressed to any desired degree. The statistical error in the exponent of (2.4) will, roughly estimated, be of the order $n^{-1/2}$ times the order of the exponent itself.

A particularly simple setup in which the statistical fluctuations may be suppressed in a controlled way is to choose a smaller set of mutually different observables $(B_1, B_2, \ldots, B_m)$, $m \ll n$, and repeat each of them sufficiently often. In other words, the sequence $(A_1, A_2, \ldots, A_n)$ is chosen to be of the form

$$(B_1, \ldots, B_1, B_2, \ldots, B_2, \ldots, B_m, \ldots, B_m). \quad (2.6)$$

If $B_\beta$ is measured $n_\beta$ times ($\sum_{\beta=1}^m n_\beta = n$), the number of measurements may be scaled up uniformly by simply replacing $n_\beta \to k \, n_\beta$ for sufficiently large $k$, while $m$ is kept constant.

Before coming to the main part of our derivation, let us describe the underlying idea. We assume that sufficiently many different observables have been chosen (details to be specified below), and for the moment we ignore $\mu(\rho)$ from (2.4). Once it is guaranteed that the statistical fluctuations are small, most experimental data (2.3) will render (2.4) very close to a family of “typical” probability distributions. For large $n$, a typical $p_\Lambda(\rho)$ may well be approximated by a Gaussian, peaked around some density matrix $\rho_\Lambda$. The latter represents the “best guess” for the unknown state, i.e. for $\tau$. Some general properties of $p_\Lambda(\rho)$ may be inferred from the fact that the exponent in (2.4) is a sum of $n$ statistically independent quantities: As $n$ increases, the typical error made by estimating the unknown state to be $\rho_\Lambda$ scales as $n^{-1/2}$. However, the quadratic form defining the “shape” of the Gaussian only depends – to leading order – on $\tau$ and on the sequence of observables chosen, i.e. it is approximately the same for all data that may reasonably occur. Hence, the distributions $p_\Lambda(\rho)$ may be viewed as translated versions of each other. In order to
have a manageable quantity at hand, we pick out the “average” distribution \( p(\rho) \),
defined by replacing the exponent in (2.4) by its expectation value (with respect to \( \tau \)). As we shall work out below in detail, it is peaked around \( \tau \). An experimentalist having performed \( n \) measurements and having inserted the data (2.3) into (2.4) will thus obtain a result very close to \( p_\Lambda(\rho) = p(\rho - \rho_\Lambda + \tau) \), with \( \rho_\Lambda = \tau + O(n^{-1/2}) \) being the best guess for the unknown state. The important point is now that the measure of knowledge (or uncertainty) depends only on the “shape” of the Gaussian (i.e. on the quadratic form in the exponent), but not on the location \( \rho_\Lambda \) of its center. (The typical \( \rho_\Lambda \) occurring in different runs of the experiment are distributed according to \( p(\rho) \)). It is in this sense that \( p(\rho) \) is “typical” and is asymptotically approached by \( p_\Lambda(\rho) \) as \( n \to \infty \).

We begin our derivation by considering the exponent in (2.4) as a function of the data \( a_1, \ldots a_n \) from (2.3). The probability distribution relevant for any \( a_j \) is \( w_a(\tau, A_j) \). Hence, we define

\[
p(\rho) = C' \mu(\rho) \exp \left( \sum_{j=1}^{n} R_j(\rho) \right),
\]

(2.7)

where

\[
R_j(\rho) = \sum_{a \in \text{Sp}(A_j)} w_a(\tau, A_j) \ln w_a(\rho, A_j),
\]

(2.8)

and \( C' \) is a normalization constant close to \( C \). Next, we define quantities \( \varepsilon_{ja}(\rho) \) by

\[
w_a(\rho, A_j) = \varepsilon_{ja}(\rho) + w_a(\tau, A_j)
\]

(2.9)

and write

\[
R_j(\rho) = H_j + S_j(\rho),
\]

(2.10)

where

\[
H_j = \sum_{a \in \text{Sp}(A_j)} w_a(\tau, A_j) \ln w_a(\tau, A_j)
\]

(2.11)

is the negative of the Shannon information measure of the probability distribution \( a \mapsto w_a(\tau, A_j) \) – it may be absorbed into the constant \( C' - \), and

\[
S_j(\rho) = \sum_{a \in \text{Sp}(A_j)} w_a(\tau, A_j) \ln \left( 1 + \frac{\varepsilon_{ja}(\rho)}{w_a(\tau, A_j)} \right)
\]

(2.12)
is – according to (2.10) – the negative of the relative entropy $S_j(\tau|\rho)$ of $a \mapsto w_a(\rho, A_j)$ to $a \mapsto w_a(\tau, A_j)$. Assuming $\varepsilon_{ja}(\rho)$ to be small ($\rho$ being close to $\tau$), we can expand

$$S_j(\rho) = \sum_{a \in \text{Sp}(A_j)} \left( \varepsilon_{ja}(\rho) - \frac{1}{2} \frac{\varepsilon_{ja}^2(\rho)}{w_a(\tau, A_j)} + O\left( \frac{\varepsilon_{ja}^3(\rho)}{w_a^2(\tau, A_j)} \right) \right).$$

(2.13)

The first term vanishes on account of $\sum_{a \in \text{Sp}(A_j)} w_a(\rho, A_j) = \sum_{a \in \text{Sp}(A_j)} w_a(\tau, A_j) = 1$ and the definition (2.9). The last term is somewhat delicate. It may be neglected if its denominator is non-zero and the number of measurements is sufficiently large. Hence, we would like to have $w_a(\tau, A_j) \neq 0 \ \forall \ a \in \text{Sp}(A_j)$ and $\forall \ j = 1, \ldots, n$. The simplest way to achieve this is to require

$$w_a(\tau, A) \neq 0 \ \forall \ a \in \text{Sp}(A)$$

(2.14)

for any observable $A$. With (2.2), this is equivalent to $\text{Tr}(\tau P) \neq 0$ for any (non-zero) hermitean projection $P$, which just states that $\tau$ is invertible, i.e. all eigenvalues of $\tau$ being non-zero. In finite dimensions, this is not a very drastic condition on the unknown state: It just states that $\tau$ lies in the interior of the set $\mathcal{S}$ of states. From now on, we shall assume this to be the case. Thus, omitting the last term in (2.13) may be compensated by a correction factor of the order

$$1 + O\left( \frac{\varepsilon_{ja}(\rho)}{w_a(\tau, A_j)} \right) \approx 1 + O\left( \| \rho - \tau \| \| \tau^{-1} \| \right)$$

(2.15)

or even closer to 1, $\| \|$ denoting the operator norm ($\|A\| = \max_{a \in \text{Sp}(A)} |a|$). It may therefore be neglected if $\rho$ is sufficiently close to $\tau$. We will show below that this will be the case in the region of interest.

Upon omitting the last term in (2.13) and re-inserting $\varepsilon_{ja}(\rho)$ from (2.9), we arrive at the result that – for invertible $\tau$ and after sufficiently many measurements – the desired probability density is given by

$$p(\rho) = K \mu(\rho) \exp\left( -\frac{1}{2} \sum_{j=1}^n Q(\rho, A_j) \right),$$

(2.16)

where

$$Q(\rho, A) = \sum_{a \in \text{Sp}(A)} \frac{(w_a(\rho, A) - w_a(\tau, A))^2}{w_a(\tau, A)}.$$
With $P_a$ denoting the spectral projections of $A$, this may also be written as

$$Q(\rho, A) = \sum_{a \in \text{Sp}(A)} \frac{\text{Tr}^2((\rho - \tau)P_a)}{\text{Tr}(\tau P_a)} \equiv \sum_{a \in \text{Sp}(A)} \frac{(\langle P_a \rangle_\rho - \langle P_a \rangle_\tau)^2}{\langle P_a \rangle_\tau}, \quad (2.18)$$

a quantity which plays a key role in what follows. The constant $K$ in (2.16), collecting $C'$ and the $\rho$-independent contribution (2.11), is chosen such that

$$\int_S \mathcal{D}\rho \ p(\rho) = 1. \quad (2.19)$$

The sum over the $Q$'s in the exponent of (2.16) defines a quadratic form on $S$. It may be written as

$$M(\rho) \equiv \sum_{j=1}^n Q(\rho, A_j) = (\rho - \tau|M|)\rho - \tau,$$ \quad (2.20)

where $M$ is a linear operator acting on $B_0$, the (real) vector space of hermitean linear operators with zero trace. Here $(\ldots|\ldots)$ denotes the Hilbert-Schmidt inner product

$$(\xi|\eta) = 2 \text{Tr}(\xi^\dagger \eta)$$ \quad (2.21)

for arbitrary linear operators $\xi$ and $\eta$, which induces a (real) inner product on $B_0$. (The factor 2 is just for convenience. It ensures that for $d = 2$ the matrices $\sigma_i/2$ form an orthonormal basis of $B_0$). With respect to (2.21), the operator $M$ is symmetric. We assume that there are enough independent observables among the $A_j$ so as to make $M$ invertible. (In fact, the overall set of all spectral projections $\{P_{ja}\}$ must span the complete $d^2$-dimensional space of hermitean linear operators). Hence, $M(\rho)$ is a non-degenerate quadratic form, the exponential part in (2.16) being a distribution of Gaussian type peaked around $\tau$. When the number of measurements is increased, the peak becomes arbitrarily sharp, eventually coming to lie well inside the domain in which (2.15) may be replaced by 1. To see this in more detail, we consider a “typical” $\rho$, whose “distance” from $\tau$ corresponds to the RMS (root mean square) deviation of the Gaussian

$$\|\rho_{\text{typical}} - \tau\|^2 \leq \text{Tr}(\rho_{\text{typical}}^2) \approx \text{Tr}(M^{-1}). \quad (2.22)$$

(For the second step, cf. (3.3) below). For large $n$, $\text{Tr}(M^{-1})$ becomes proportional to $n^{-1}$. Hence, $n$ may be chosen large enough so as to make (2.15) arbitrarily close
to 1 for any “typical” $\rho$. With increasing $n$, the approximation becomes arbitrarily accurate.

In case of choosing $m$ observables $B_1, \ldots, B_m$ according to the scheme (2.6), and performing $n_\beta$ measurements of $B_\beta$, (2.18) and (2.20) combine into

$$M(\rho) = \sum_{\beta=1}^{m} n_\beta Q(\rho, B_\beta) = (\rho - \tau |M| \rho - \tau). \quad (2.23)$$

In order to render $M$ invertible, we must have $m \geq d+1$. The lower bound $m = d+1$ may only be attained if the overall set of all spectral projections $\{P_\beta\}$ spans the (real) vector space of hermitean linear operators, which implies that each $B_\beta$ has only non-degenerate eigenvalues. This formula will turn out particularly useful later on.

Now we have to say some words about the à priori probability distribution $\mu$ contained in (2.16). We mainly focus on situations where nothing – or very few – is known about $\tau$ before the measurements are carried out. One would then choose $\mu$ to be spread over the whole of $S$. Consequently, the functional dependence of $\mu(\rho)$ is dominated by the peak of the Gaussian. In particular, if $\mu$ is continuous at $\rho = \tau$, $\mu(\rho)$ may effectively be replaced by $\mu(\tau)$ for large $n$. Hence, it is justified to ignore this factor, and we will set $\mu(\rho) \equiv 1$ for the rest of this paper.

Finally, the region of integration in (2.19) may effectively be replaced by the set of hermitean linear operators with trace unity, which is isomorphic to $\mathbb{R}^{d^2-1}$. Thus we end up with the standard normalized Gaussian

$$p(\rho) = \sqrt{\frac{\det M}{(2\pi)^{d^2-1}}} \exp \left( -\frac{1}{2} (\rho - \tau |M| \rho - \tau) \right), \quad (2.24)$$

where $M$ is the linear operator $M$ as defined in (2.20) or in the more convenient form (2.23). This operator – depending only on $\tau$ and on the sequence of observables – is thus the key object allowing us to quantify the gain of knowledge in terms of a single numerical measure. We recall that, when the experimentalist inserts the measurement outcome data (2.3) into (2.4), he will obtain a probability distribution very close to a translated version of $p(\rho)$, i.e.

$$p_\Lambda(\rho) = \sqrt{\frac{\det M}{(2\pi)^{d^2-1}}} \exp \left( -\frac{1}{2} (\rho - \rho_\Lambda |M| \rho - \rho_\Lambda) \right), \quad (2.25)$$

where $\rho_\Lambda$ differs from $\tau$ by $O(n^{-1/2})$. 

9
3 Measures of knowledge and best strategies in general

The distribution (2.24) is determined by the quadratic form (2.20) or (2.23), i.e. by the linear operator \( M \) on the (real) vector space of hermitean linear operators with trace 0. As described above, \( M \) contains all the information necessary to work out the experimentalist’s knowledge (or uncertainty) about the unknown state, once he knows the data. The only freedom that is left for him is to choose the sequence of observables \( A_j \). However, prior to searching a strategy (i.e. a choice of observables) that maximizes this knowledge, we first have to specify how the “knowledge about the unknown state” – or, conversely, the “uncertainty about the unknown state” – is quantified. The answer depends on which feature of the unknown state is required. We consider two possible approaches:

a.) Volume in \( S \):
The peak of the Gaussian (2.24) occupies a “volume” in the set \( S \) of states of the order
\[
V = (\det M)^{-1/2},
\]
which may be considered as a measure of uncertainty about \( \tau \). This is not identical with, but plays a similar role as Wootters and Fields’ “uncertainty volume” [1], before the average over the possible unknown states is performed. It corresponds to the information theoretic notion of knowledge since it is related monotonously to the negative of the Shannon information measure
\[
H = \int_S \mathcal{D} \rho \ p(\rho) \ln p(\rho) = -\frac{d^2-1}{2} + \frac{1}{2} \ln \left( \frac{\det M}{(2\pi)^{d^2-1}} \right).
\]
A best strategy based on this measure (a best “volume oriented strategy”) is one for which \( \det M \) is maximal for given \( n \).

b.) Distance from \( \tau \):
The RMS (root mean square) deviation of the distribution (2.24) is given by
\[
D^2 = (\Delta \rho)^2 \equiv \int_S \mathcal{D} \rho \ p(\rho) \ Tr \left( (\rho - \tau)^2 \right) = Tr(M^{-1}).
\]
It represents the uncertainty about the unknown state as measured in terms of the mean “distance squared” \( Tr((\rho - \tau)^2) \) in the space \( S \) of states and defines a
“length” scale $D$. A best strategy based on this measure (a best “distance oriented strategy”) is one for which $\text{Tr}(\mathcal{M}^{-1})$ is minimal for given $n$.

It is easy to see that any best strategy based on maximizing $\det\mathcal{M}$ or minimizing $\text{Tr}(\mathcal{M}^{-1})$ necessarily has to use observables $A_j$ with non-degenerate eigenvalues only. At the level of our formalism, this feature may be traced back to the properties of the quadratic form $M(\rho)$, as given by (2.20) or (2.23), and its constituents $Q(\rho, A)$ as defined in (2.17) and (2.18): We first note that $M(\rho)$ is a sum, each term stemming from a particular measurement. $Q(\rho, A)$ may thus be considered as a measure of how our knowledge increases (on the average) by a measurement of $A$. $M(\rho)$ has the important property that the contribution of an observable $A$ will be the larger, the more spectral projections $A$ possesses: Let $A$ be one of our observables measured, and suppose it possesses a degenerate eigenvalue $a$. The corresponding eigenspace (the image of the spectral projection $P_a$) thus has dimension greater than 1. Suppose now that the measurement of $A$ is replaced by the measurement of another observable $A'$, constructed from $A$ by replacing $aP_a \rightarrow a'P_{a'} + a''P_{a''}$ in the spectral decomposition of $A$ (where $a' \neq a''$, both numbers being different from the other eigenvalues of $A$, and $P_{a'}$, $P_{a''}$ being orthogonal projections dividing the eigenspace into a direct sum: $P_a = P_{a'} + P_{a''}$). We can consider $A'$ as a “refinement” of $A$. Now we compare the two corresponding quantities $M(\rho)$ and $M'(\rho)$. Explicit computation reveals

$$M'(\rho) - M(\rho) = Q(\rho, A') - Q(\rho, A) = \left( \frac{\text{Tr}(\tau P_{a'}) \text{Tr}\left((\rho - \tau)P_{a''}\right) - \text{Tr}(\tau P_{a''}) \text{Tr}\left((\rho - \tau)P_{a'}\right)}{\text{Tr}(\tau P_{a'}) \text{Tr}(\tau P_{a''}) \text{Tr}\left(\tau(P_{a'} + P_{a''})\right)} \right)^2,$$

which represents a semi-positive quadratic form by its own. Consequently, we have $\det\mathcal{M}' \geq \det\mathcal{M}$ and $\text{Tr}(\mathcal{M}'^{-1}) \leq \text{Tr}(\mathcal{M}^{-1})$, while the total number $n$ of measurements has not been changed. The same procedure may be repeated until all degenerate eigenvalues of all observables $A_j$ have disappeared. (The same behaviour is expected for any other reasonable measure of knowledge).

By construction, the best strategies depend on the unknown state $\tau$. Hence, one may object that when $\tau$ is unknown, the experimentalist does not know how to choose his observables. On the other hand, when inserting the outcomes of a relatively small number of measurements of arbitrary observables into (2.4), one
obtains a first rough estimate of $\tau$. Next, one chooses observables according to a best strategy as if the estimate in fact coincides with the unknown state. After some runs of this type (or even after each measurement) one determines a better estimate for $\tau$ and re-adjusts the observables. This procedure is iterated and will, for increasing $n$, approach the effectiveness of a best strategy.

4 The two-dimensional case

Let us now study the case $d = 2$ in some detail. Since the states and observables on a two-dimensional Hilbert space admit a simple geometric representation, we can be more explicit than in the case of general $d$. The set of all density matrices may be parametrized as

$$\rho(\vec{a}) = \frac{1}{2} (1 + \vec{a} \vec{\sigma}) \quad \text{with} \quad |\vec{a}| \leq 1,$$

where $\vec{\sigma}$ represents three observables obeying the Pauli spin matrix algebra, and $\vec{a} \in \mathbb{R}^3$. Pure states are characterized by $|\vec{a}| = 1$, the tracial state is given by $\vec{a} = 0$. The space $\mathcal{S}$ of states is thus represented by the unit ball in $\mathbb{R}^3$. The natural measure $\mathcal{D}\rho$ on $\mathcal{S}$ is the Euclidean volume element $d^3a$.

Now let us look at observables. Any hermitean linear operator may be written as $a \mathbf{1} + \vec{c} \vec{\sigma}$ with $a \in \mathbb{R}$ and $\vec{c} \in \mathbb{R}^3$. Leaving aside multiples of the identity and irrelevant multiplicative factors, we confine ourselves to measuring observables of the type

$$B(\vec{c}) = \vec{c} \vec{\sigma} \quad \text{with} \quad |\vec{c}| = 1.$$  

The spectrum of any such operator is $\{-1, 1\}$. The spectral projection corresponding to the eigenvalue $b \in \{-1, 1\}$ of $B(\vec{c})$ takes the convenient form $P_b = \frac{1}{2} (1 + b \vec{c} \vec{\sigma})$, and the measurement outcome probabilities for this observable in the state $\rho(\vec{a})$ read

$$w_b(\rho(\vec{a}), B(\vec{c})) = \frac{1}{2} (1 + b \vec{a} \vec{c}).$$

We now specify our sequence of observables according to the scheme (2.6): We choose $m$ unit vectors $\vec{c}_\beta (\beta = 1, \ldots m)$ and perform $n_\beta$ measurements of each $B_\beta \equiv B(\vec{c}_\beta)$. The total number of measurements is therefore $n = \sum_{\beta=1}^m n_\beta$. The unknown state shall be represented the parameter value $\vec{u}$, i.e.

$$\tau \equiv \rho(\vec{u}),$$

12
and $p(\rho)$ is written as $p(\vec{a})$. Using (2.23), a short computation reveals that the probability distribution (2.24) is given by

$$p(\vec{a}) = \sqrt{\frac{\det M}{(2\pi)^3}} \exp\left( -\frac{1}{2} (\vec{a} - \vec{u})^T \mathcal{M} (\vec{a} - \vec{u}) \right),$$

where $\mathcal{M}$ is the $3 \times 3$ matrix with components

$$\mathcal{M}_{rs} = \sum_{\beta=1}^{m} \frac{n_\beta}{1 - (\vec{u} \cdot \vec{c}_\beta)^2} c_{\beta r} c_{\beta s},$$

$c_{\beta r}$ being the components of the vector $\vec{c}_\beta$, with $r$ and $s$ ranging from 1 to 3. Starting with this expression, we will now tackle the problem of finding all best strategies for the determination of the unknown state $\rho(\vec{u})$.

5 Best strategies for $d = 2$

The form of (4.6) shows that we must have $m \geq 3$, and the sequence of vectors $\vec{c}_\beta$ must contain three linearly independent elements (otherwise $\mathcal{M}$ would not be invertible). In other words, the $m \times 3$ matrix defined by the components $c_{\beta r}$ must have rank 3. According to the two measures of knowledge as discussed in section 3, we consider the two cases of maximizing $\det \mathcal{M}$ and minimizing $\text{Tr}(\mathcal{M}^{-1})$.

a.) Maximizing $\det \mathcal{M}$:

We first consider the volume oriented approach, i.e. the case when the “volume” $V$ in $\mathcal{S}$ occupied by the peak of the Gaussian (4.5) serves as a measure for the uncertainty about the unknown state. Let us fix $n$ (and, for the moment, $m$) and ask for which configurations $(n_\beta, \vec{c}_\beta)$ the determinant of $\mathcal{M}$ is maximal under the subsidiary conditions $\sum_{\beta=1}^{m} n_\beta = n$ and $|\vec{c}_\beta| = 1 \forall \beta$. Introducing Lagrange multipliers $c, C_\beta$, the corresponding unconstrained problem is to maximize

$$\mathcal{F} = \ln \det \mathcal{M} - c \sum_{\beta=1}^{m} n_\beta - \frac{1}{2} \sum_{\beta=1}^{m} C_\beta c^2_\beta$$

with respect to the variables $(n_\beta, \vec{c}_\beta, c, C_\beta)$. The logarithm is used just for convenience: This form allows us to apply the general formula $\partial (\ln \det \mathcal{M}) = \text{Tr}(\mathcal{M}^{-1} \partial \mathcal{M})$, where $\partial$ stands for any derivative $\partial/\partial c_{\beta r}$ or $\partial/\partial n_\beta$. Now we choose the coordinates
in \( \mathbb{R}^3 \) such that \( \mathcal{M} \) is diagonal in the maximizing configuration. This choice is possible because \( \mathcal{M} \) is a hermitean matrix, and it causes all non-diagonal elements to drop out of the problem. Differentiation with respect to \( n_\beta \) and \( c_\beta r \) leads to the set of equations

\[
\frac{1}{1 - (\vec{u} \vec{c}_\beta)^2} \sum_{s=1}^{3} \frac{c_{\beta s}^2}{\mathcal{M}_{ss}} = c \quad (5.2)
\]

\[
\frac{2 n_\beta c_\beta r}{1 - (\vec{u} \vec{c}_\beta)^2} \frac{\mathcal{M}_{rr}}{2} + \frac{2 n_\beta (\vec{u} \vec{c}_\beta) u_r}{1 - (\vec{u} \vec{c}_\beta)^2} \sum_{s=1}^{3} \frac{c_{\beta s}^2}{\mathcal{M}_{ss}} = C_\beta c_\beta r \quad (5.3)
\]

whose combination yields

\[
\frac{2 n_\beta}{1 - (\vec{u} \vec{c}_\beta)^2} \left( \frac{c_\beta r}{\mathcal{M}_{rr}} + (\vec{u} \vec{c}_\beta) u_r c \right) = C_\beta c_\beta r \quad (5.4)
\]

Multiplying this equation by \( c_\beta r \), summing over \( r \) and using (5.2) and \( |\vec{c}_\beta| = 1 \ \forall \beta \) gives

\[
C_\beta = \frac{2 n_\beta c}{1 - (\vec{u} \vec{c}_\beta)^2} \quad (5.5)
\]

Multiplying (5.2) by \( n_\beta \), summing over \( \beta \) and using (4.6) and \( \sum_{\beta=1}^{m} n_\beta = n \) leads to

\[
c = \frac{3}{n} \quad (5.6)
\]

Upon inserting these last two expressions into (5.4), we find

\[
c_\beta r \left( \frac{1}{\mathcal{M}_{rr}} - \frac{3}{n} \right) + \frac{3}{n} (\vec{u} \vec{c}_\beta) u_r = 0 \quad (5.7)
\]

Since the \( m \times 3 \) matrix defined by \( c_\beta r \) has rank 3 – as argued at the beginning of this section –, the term \( (\mathcal{M}_{rr})^{-1} - 3 n^{-1} \) must vanish for at least two values of \( r \) (otherwise one could divide by these terms for two or three values of \( r \) and conclude that \( c_\beta r \) has rank less than 3). We may choose the coordinates of \( \mathbb{R}^3 \) such that these values are \( r = 1 \) and 2. Hence, \( \mathcal{M}_{11} = \mathcal{M}_{22} = \frac{1}{3} n \), which implies \( u_1 = u_2 = 0 \), \( \vec{u} \vec{c}_\beta = u_3 c_\beta 3 \) and \( u_3^2 = \vec{u}^2 \). Equation (5.7) thus shrinks to the statement that \( \mathcal{M}_{33} = \frac{1}{3} n (1 - \vec{u}^2)^{-1} \), and the remaining equation (5.2) is automatically satisfied. In this way we arrive at the following
Lemma 1:
For given \( \vec{u} \) and \( n \), the configuration \((m, n_\beta, \vec{c}_\beta)\) maximizes \( \text{det} \mathcal{M} \) under the subsidiary conditions \( \sum_{\beta=1}^{n} n_\beta = n \) and \( |\vec{c}_\beta| = 1 \ \forall \beta \) if and only if

(i) \( \vec{u} \) is an eigenvector of \( \mathcal{M} \) associated with the eigenvalue \( \frac{1}{3}n(1 - \vec{u}^2)^{-1} \), and

(ii) the two other eigenvalues of \( \mathcal{M} \) are both equal to \( \frac{1}{3}n \).

The second statement implies that \( \mathcal{M} \) acts proportional to the identity in the subspace orthogonal to \( \vec{u} \). The value of \( \text{det} \mathcal{M} \) in the maximizing configuration is given by

\[
(\text{det}\mathcal{M})_{\text{max}} = \left( \frac{n}{3} \right)^3 \frac{1}{1 - \vec{u}^2},
\]

or, expressed in terms of the “volume” \( V = (\text{det}\mathcal{M})^{-1/2} \) occupied by the peak of the Gaussian,

\[
V_{\text{min}} = \left( \frac{3}{n} \right)^{3/2} \sqrt{1 - \vec{u}^2}. \tag{5.9}
\]

Any configuration satisfying (i) and (ii) represents a “best strategy”, and all these strategies work equally well, because (5.8) depends only on \( n \) and \( \vec{u} \), but not on any details of the configuration \((m, n_\beta, \vec{c}_\beta)\). The simplest strategy is to choose \( m = 3 \) and let \( \{\vec{c}_1, \vec{c}_2, \vec{c}_3\} \) be an orthonormal basis of \( \mathbb{R}^3 \) such that one of these vectors (\( \vec{c}_3 \), say) is parallel to \( \vec{u} \). In this strategy, we must have \( n_1 = n_2 = n_3 = \frac{1}{3}n \), i.e. all three observables \( B_\beta \equiv B(\vec{c}_\beta) \) are measured equally often.

b.) Minimizing \( \text{Tr}(\mathcal{M}^{-1}) \):

The distance oriented approach, i.e. the case when the mean “distance squared” from the center of the Gaussian (4.5) serves as a measure for the uncertainty about the unknown state, is treated similarly. Formally, the problem consists of minimizing

\[
\mathcal{F} = \text{Tr}(\mathcal{M}^{-1}) + c \sum_{\beta=1}^{m} n_\beta + \frac{1}{2} \sum_{\beta=1}^{m} C_\beta \vec{c}_\beta^2, \tag{5.10}
\]

where \( c \) and \( C_\beta \) are Lagrange multipliers. We again choose the coordinates in \( \mathbb{R}^3 \) such that \( \mathcal{M} \) is diagonal in the minimizing configuration and use the general formula \( \partial(\text{Tr}(\mathcal{M})^{-1}) = -\text{Tr}(\mathcal{M}^{-1}(\partial \mathcal{M})(\mathcal{M}^{-1})) \), where \( \partial \) stands for \( \partial/\partial c_{\beta r} \) and \( \partial/\partial n_\beta \). Differentiation yields a set of equations that look like (5.2)–(5.3), except that the diagonal elements \( \mathcal{M}_{rr} \) and \( \mathcal{M}_{ss} \) are replaced by their squares, and the same applies.
to the analogue of (5.4). Equation (5.5) appears without change, but the analogue of (5.6) now takes the form
\[ c = \frac{1}{n} \sum_{s=1}^{3} \frac{1}{M_{ss}}, \]  
(5.11)
due to an additional appearance of \((M_{ss})^{-1}\) in the analogue of (5.2). Hence, the analogue of (5.7) becomes
\[ c_{\beta r} \left( \frac{1}{M_{rr}^2} - c \right) + c(\bar{u}_{\beta\bar{c}_\beta}) u_r = 0 \]  
(5.12)
with \(c\) from (5.11). Following the same logic as before, the term \((M_{rr})^{-2} - c\) must vanish for at least two values of \(r\) (which we choose to be 1 and 2). This implies \(u_1 = u_2 = 0\) and
\[ \frac{1}{M_{11}^2} = \frac{1}{M_{22}^2} = c \quad \frac{1}{M_{33}^2} = c (1 - \bar{u}^2). \]  
(5.13)
Combining these equations with (5.11), we may easily compute the diagonal elements \(M_{rr}\), i.e. the eigenvalues of \(M\) (to be displayed below). The remaining equation – the analogue of (5.2) – is then automatically satisfied. Our result thus reads:

**Lemma 2:**

For given \(\bar{u}\) and \(n\), the configuration \((m, n_\beta, \bar{c}_\beta)\) minimizes \(\text{Tr}(M^{-1})\) under the subsidiary conditions \(\sum_{\beta=1}^{n} n_\beta = n\) and \(|\bar{c}_\beta| = 1 \forall \beta\) if and only if

(i) \(\bar{u}\) is an eigenvector of \(M\) associated with the eigenvalue
\[ \frac{n}{(2 + \sqrt{1 - \bar{u}^2})\sqrt{1 - \bar{u}^2}}, \]  
(5.14)
and

(ii) the two other eigenvalues of \(M\) are both equal to
\[ \frac{n}{2 + \sqrt{1 - \bar{u}^2}}. \]  
(5.15)
The second statement implies that \(M\) acts proportional to the identity in the subspace orthogonal to \(\bar{u}\). The value of \(\text{Tr}(M^{-1})\) in the minimizing configuration is given by
\[ D_{\min}^2 \equiv \text{Tr}(M^{-1})_{\min} = \frac{1}{n} \left(2 + \sqrt{1 - \bar{u}^2}\right)^2. \]  
(5.16)
Any configuration satisfying (i) and (ii) represents a “best strategy”, and all these strategies work equally well. The simplest one is to choose $m = 3$ and let \{\vec{c}_1, \vec{c}_2, \vec{c}_3\} be an orthonormal basis of $\mathbb{R}^3$ such that one of these vectors (\vec{c}_3, say) is parallel to $\vec{u}$. The numbers of measurements performed of any of the three observables $B_\beta \equiv B(\vec{c}_\beta)$ must now be chosen as

\[
n_1 = n_2 = \frac{n}{2 + \sqrt{1 - \vec{u}^2}} \quad n_3 = \frac{n \sqrt{1 - \vec{u}^2}}{2 + \sqrt{1 - \vec{u}^2}},
\]

and they correctly sum up to $n$. The observable aligned with $\vec{u}$ thus needs less measurements than the others.

Comparing a.) and b.):
The knowledge about the unknown state after $n$ optimally chosen measurements is given by the volume (5.9) and the length squared (5.16), respectively. For small $|\vec{u}|$, these two methods work roughly equally well. In both cases, the three eigenvalues of $M$ are approximately of the same order, the spread of the Gaussian thus being roughly the same in all directions in $\mathcal{S}$. If, however, $|\vec{u}|$ is close to 1 (i.e. $\tau$ being almost pure), one eigenvalue of $M$ becomes large in both cases, thus causing the peak to be spread only very little in the direction of $\vec{u}$. In this situation the “volume” oriented approach is more efficient: In the limit $|\vec{u}| \to 1$ for fixed $n$ we have $\mathcal{V}_{\min} \to 0$, whereas $D_{\min}^2 \to 4n^{-1}$.

In both cases, the strategy works as follows: When inserting the outcomes of a relatively small number of measurements of arbitrary observables into (2.4), one obtains a first rough estimate of $\tau$, i.e. of $\vec{u}$. Next one chooses an orthonormal basis \{\vec{c}_1, \vec{c}_2, \vec{c}_3\} of $\mathbb{R}^3$ such that $\vec{c}_3$ is parallel to the best guess of $\vec{u}$. One then measures the three corresponding observables $B(\vec{c}_\beta)$ (the relative number of measurements depending on whether $\mathcal{V}$ or $D^2$ represents the measure of uncertainty). After some runs of this type (or even after each measurement) one determines a better guess of $\vec{u}$ and re-adjust the three vectors accordingly ($\vec{c}_3^{\text{new}}$ being aligned with the new guess of $\vec{u}$, and $\vec{c}_1^{\text{new}}$ and $\vec{c}_2^{\text{new}}$ being as close to $\vec{c}_1$ and $\vec{c}_2$ as possible). This procedure is iterated and will, for increasing $n$, converge to an orthonormal basis representing a “best strategy” as determined above. In other words: for sufficiently large $n$, we expect the bounds (5.9) or (5.16), respectively, to be approached arbitrarily well.
6 Comparison of strategies in higher dimensions

In this section we consider the case of higher dimensional Hilbert spaces. After presenting a generally applicable method to improve strategies, we show how concrete strategies may be constructed. It turns out that a strategy based on mutually unbiased (complementary) observables is not always optimal. Concluding, we give some remarks about the infinite dimensional case.

General formalism

We now turn to higher dimensions. Let the dimension $d$ of $\mathcal{H}$ be arbitrary. By $\mathcal{B}$, we denote the (complex) vector space of all linear operators on $\mathcal{H}$, endowed with the Hilbert-Schmidt inner product (2.21). The latter makes $\mathcal{B}$ a $d^2$-dimensional Hilbert space by its own. We will use a bra-ket-notation for this space, using round brackets, i.e. $|\xi\rangle\langle\eta|$ representing the linear operator $\mathcal{B} \to \mathcal{B}$ sending $\zeta \mapsto |\xi\rangle\langle\eta|\zeta$ or, equivalently, $\zeta \mapsto 2\text{Tr}(\eta^\dagger\zeta)\xi$. The determinant and trace of linear operators $\mathcal{B} \to \mathcal{B}$ will be denoted by the symbols $\det_\otimes$ and $\text{Tr}_\otimes$, respectively. Furthermore, we need a component formalism for operators of this type. If $\{e_I|I = 1, \ldots d\}$ is an orthonormal basis of $\mathcal{H}$, the linear operators ("matrix units")

$$e_{IJ} \equiv |e_I\rangle\langle e_J| : \mathcal{H} \to \mathcal{H}$$

(6.1)

form a basis of $\mathcal{B}$, satisfying $(e_{IJ}|e_{KL}) = 2\delta_{IK}\delta_{JL}$. Along with the expansion of elements $\xi \in \mathcal{B}$ as

$$\xi = \sum_{I,J} \xi_{IJ} e_{IJ} \equiv \sum_{I,J} |e_I\rangle\xi_{IJ}\langle e_J| \quad \text{with} \quad \xi_{IJ} = \langle e_I|\xi|e_J\rangle,$$

(6.2)

any linear operator $\mathcal{A} : \mathcal{B} \to \mathcal{B}$ may be written as

$$\mathcal{A} = \frac{1}{2} \sum_{I,J,K,L} |e_{IJ}\rangle\mathcal{A}_{IJ,KL}(e_{KL}|$$

with $\mathcal{A}_{IJ,KL} = \frac{1}{2} (e_{IJ}|\mathcal{A}|e_{KL}).$ (6.3)

In terms of these components, the action of $\mathcal{A}$ is represented by a matrix multiplication. When understanding the values of the double index $IJ$ by a single index $r$, the components $\mathcal{A}_{IJ,KL}$ explicitly define a $d^2 \times d^2$ matrix representation $\mathcal{A}_r$, in which the determinant and the trace take their usual form. If $\mathcal{A} = |\xi\rangle\langle\eta|$, we have

$$\mathcal{A}_{IJ,KL} = 2\xi_{IJ} \eta^*_{KL}.$$ (6.4)
The orthogonal projection onto the normalized element \((2d)^{-1/2}\mathbf{1}\)

\[
P = \frac{1}{2d} \mathbf{1}(\mathbf{1}) : \mathcal{B} \to \mathcal{B}
\]

(\mathbf{1} denoting the unit operator on \(\mathcal{H}\)) has components \(P_{IJ,KL} = d^{-1}\delta_{IJ}\delta_{KL}\).

By \(\mathcal{B}_0\), we denote the subset of \(\mathcal{B}\) consisting of all hermitean linear operators with zero trace. It is a real vector space of dimension \(d^2 - 1\), and the Hilbert-Schmidt inner product for any pair of its elements is real. The determinant and trace of linear operators \(\mathcal{B}_0 \to \mathcal{B}_0\) are denoted by the symbols \(\det\) and \(\Tr\), respectively.

We now consider a strategy based on the scheme (2.6), i.e. a collection \(B_\beta\) \((\beta = 1, \ldots m)\) of operators, such that each \(B_\beta\) is measured \(n_\beta\) times in a copy of the system, and \(\sum_{\beta=1}^{m} n_\beta = n\). We assume \(n_\beta \gg 1\) for each \(\beta\). (As noted above, sufficiently large \(n\) may be achieved by replacing \(n_\beta \to kn_\beta\) for sufficiently large \(k\), while keeping \(m\) constant.) The key object describing the quality of the strategy is the symmetric linear operator \(\mathcal{M} : \mathcal{B}_0 \to \mathcal{B}_0\) as defined in (2.23) and appearing in the Gaussian (2.24). As may be read off from (2.23) and (2.18), any observable \(A\) provides a contribution

\[
\mathcal{Q}(A) = \frac{1}{2} \sum_{a \in \text{Sp}(A)} \frac{|P_a\rangle\langle P_a|}{(\tau|P_a)},
\]

where \(P_a\) is the spectral projection of \(A\) with respect to the eigenvalue \(a\). However, when written in the above form, any such object is a hermitean linear operator \(\mathcal{Q}(A) : \mathcal{B} \to \mathcal{B}\) that does not leave \(\mathcal{B}_0\) invariant. Its components are given by

\[
\mathcal{Q}_{IJ,KL}(A) = \sum_{a \in \text{Sp}(A)} \frac{P_{a,IJ}P_{a,KL}^*}{(\tau|P_a)},
\]

where \(P_{a,IJ}\) are the components of \(P_a\). From now on, we assume the orthonormal basis \(\{e_i\}\) to consist of eigenvectors of \(\tau\). As a consequence, the matrix \(\tau_{IJ}\) is diagonal, and the denominator in (6.7) is \((\tau|P_a) = 2\sum_I \tau_{II}P_{a,II}\).

When summing up (6.6) for the observables \(B_\beta\), we arrive at a hermitean operator acting on \(\mathcal{B}\). It will turn out convenient to generalize it to a family of operators \(\mathcal{M}_\circ(\alpha) : \mathcal{B} \to \mathcal{B}\), defined as

\[
\mathcal{M}_\circ(\alpha) = \sum_{\beta=1}^{m} n_\beta \mathcal{Q}(B_\beta) + \alpha P,
\]
where \( P \) is given by (6.5). Since \((1|\xi) \equiv 2 \text{Tr}(\xi) = 0\) for any traceless \( \xi \), we have \((\xi|M_0(\alpha)|\eta) = (\xi|M|\eta)\) for all \( \xi, \eta \in B_0 \). This establishes the relation between \( M_0(\alpha) \) and the original object \( M : B_0 \to B_0 \).

We will now express our two measures of knowledge, (3.1) and (3.3), in terms of \( M_0(\alpha) \). Since \( P \) is the (one-dimensional) hermitean projection onto the orthogonal complement of \( B_0 \), (6.8) tells us that

\[
\det \circ M_0(\alpha) = \alpha \det M + \text{terms independent of } \alpha. \tag{6.9}
\]

From this it follows

\[
\det M = \lim_{\alpha \to \infty} \frac{\det \circ M_0(\alpha)}{\alpha}, \tag{6.10}
\]

and analogously we conclude

\[
\text{Tr}(M^{-1}) = \lim_{\alpha \to \infty} \text{Tr}_\circ \left( M_0(\alpha)^{-1} \right). \tag{6.11}
\]

These two quantities is all we need in order to compare strategies.

**Improving strategies**

We now return to the problem of optimizing measurement strategies. Given some particular strategy characterized by \( M_0(\alpha) \), we show how to construct another strategy which is at least as good as the original one.

For any observable \( B_\beta \), we consider the family \( B'_\beta(\varphi) = e^{i\varphi\tau}B_\beta e^{-i\varphi\tau} \). We may think of unitarily “rotating” \( B_\beta \) within \( B \) in such a way that the unknown state \( \tau \) is invariant. When selecting an arbitrary value of \( \varphi \), and replacing the observables \( B_\beta \) by \( B'_\beta(\varphi) \), we obtain a strategy that is obviously equivalent to the original one. Denoting its associated family of \( M \)-operators by \( M'_0(\alpha, \varphi) \), we have

\[
\det \circ M'_0(\alpha, \varphi) = \det \circ M_0(\alpha), \tag{6.12}
\]

\[
\text{Tr}_\circ \left( M'_0(\alpha, \varphi)^{-1} \right) = \text{Tr}_\circ \left( M_0(\alpha)^{-1} \right), \tag{6.13}
\]

for all \( \alpha \). We will now construct a further strategy out of these equivalent ones: We distribute the \( n_\beta \) measurements originally reserved for \( B_\beta \) among members of the family \( B'_\beta(\varphi) \). Technically, we introduce a probability distribution \( \varphi \mapsto f(\varphi) \) according to which a value for \( \varphi \) is thrown in order to determine the observable
$B'_\beta(\varphi)$ to be measured next. In a first step we may think of $f$ as a discrete distribution (admitting only particular values for $\varphi$). However, for sufficiently large $n_\beta$, this may arbitrarily well be approximated by allowing $f$ to be a continuous distribution. Hence, the average number of measurements carried out for observables $B'_\beta(\varphi)$ satisfying $\varphi_0 \leq \varphi \leq \varphi_0 + d\varphi$ will be $n_\beta f(\varphi_0)d\varphi$.

It may of course happen that different observables $B_\beta$ effectively play the same role in the new strategy. This will happen if they are already “rotated” versions of each other, e.g. if $B_2 = e^{i\varphi \tau} B_1 e^{-i\varphi \tau}$ and $f(\varphi) \neq 0$ for some $\varphi$. In this case, the new strategy is effectively generated by a smaller set of observables than contained in the original strategy (while the number of different observables actually measured will in general increase).

By construction, the operator $\mathcal{M}'_\odot(\alpha)$ for the new strategy is given by the average

$$\mathcal{M}'_\odot(\alpha) = \int d\varphi f(\varphi) \mathcal{M}'_\odot(\alpha, \varphi). \quad (6.14)$$

Since $\mathcal{M} \mapsto \mathcal{M}^{-1}$ and $\mathcal{M} \mapsto \ln \mathcal{M}$ are operator convex functions, it follows from the Peierls-Bogoliubov inequality that

$$\det_\odot \mathcal{M}'_\odot(\alpha) \equiv \exp \left( \Tr_\odot (\ln \mathcal{M}'_\odot(\alpha)) \right) \geq \det_\odot \mathcal{M}_\odot(\alpha), \quad (6.15)$$

$$\Tr_\odot (\mathcal{M}'_\odot(\alpha)^{-1}) \leq \Tr_\odot (\mathcal{M}_\odot(\alpha)^{-1}), \quad (6.16)$$

where have taken into account (6.12) and (6.13). These inequalities survive the limits (6.10) and (6.11), so that we conclude

$$\det \mathcal{M}' \geq \det \mathcal{M}, \quad (6.17)$$

$$\Tr (\mathcal{M}'^{-1}) \leq \Tr (\mathcal{M}^{-1}). \quad (6.18)$$

With respect to the measures of knowledge in both the volume and the distance oriented approach, the new strategy is better than (or equally well as) the original one.

Let us now compute the operator $\mathcal{M}'_\odot(\alpha)$ for the new strategy more explicitly. The spectral projection of $B'_\beta(\varphi)$ with respect to the eigenvalue $a$ is given by $P'_\beta a(\varphi) = e^{i\varphi \tau} P_\beta a e^{-i\varphi \tau}$. Hence, $(\tau | P'_\beta a(\varphi)) = (\tau | P_\beta a(\varphi))$ for any $\varphi$, so that nothing changes in the denominators in (6.6) and (6.7). Since the basis vectors $e_I$ are eigenvectors of $\tau$, the components of the new spectral projections become $P'_{\beta a, IJ}(\varphi) \equiv$
\[ \langle e_I | P'_{\beta a}(\varphi) | e_J \rangle = e^{i\varphi(\tau_{II} - \tau_{JJ})} \langle e_I | P_{\beta a} | e_J \rangle \equiv e^{i\varphi(\tau_{II} - \tau_{JJ})} P_{\beta a, JJ}. \]  
Thus, when computing the components \( M'_{\otimes, II, JJ}(\alpha) \), the integral over \( \varphi \) is to be taken over 
\[ e^{i\varphi(\tau_{II} - \tau_{JJ} - \tau_{KK} + \tau_{LL})}. \]  
\( (6.19) \)

In order to give it a simple form, we choose \( f \) such that the integral over these expressions is only non-zero if \( I = J \) and \( K = L \) or \( I = K \) and \( J = L \). This gives 
\[ \int d\varphi f(\varphi) e^{i\varphi(\tau_{II} - \tau_{JJ} - \tau_{KK} + \tau_{LL})} = \delta_{IJ} \delta_{KL} + \delta_{IK} \delta_{JL} - \delta_{IJKL}, \]  
\( (6.20) \)

where \( \delta_{IJKL} = 1 \) if all four indices agree, and 0 otherwise. Strictly speaking, this is only possible if the eigenvalues \( \tau_{II} \) are sufficiently different from each other. If this is not the case, one may choose some appropriate hermitean operator \( \xi \) commuting with \( \tau \) and redefine \( B'_{\beta}(\varphi) = e^{i\varphi} B_{\beta} e^{-i\varphi} \xi \). Choosing the eigenvalues of \( \xi \) to have only rational quotients, there is always a finite interval for the \( \varphi \)-integration such that \( (6.20) \) is valid with \( f(\varphi) = \text{const} \). Otherwise one would have to use the invariant mean 
\[ \int d\varphi f(\varphi) \ldots \longrightarrow \lim_{T \to \infty} \frac{1}{2T} \int_{-T}^{T} d\varphi \ldots \]  
\( (6.21) \)

With the choice \( (6.20) \), the transition from the old to the new strategy is simply achieved by 
\[ M'_{\otimes, II, JJ}(\alpha) = (\delta_{IJ} \delta_{KL} + \delta_{IK} \delta_{JL} - \delta_{IJKL}) M_{\otimes, II, JJ}(\alpha). \]  
\( (6.22) \)

In effect, the average over equivalent strategies has cut off some of the original components, but has left the remaining ones \( (M'_{\otimes, II, JJ}(\alpha) \text{ and } M'_{\otimes, I, I, J}(\alpha)) \) unchanged.

Due to the blockform of \( (6.22) \), any of the operators \( M'_{\otimes}(\alpha) \) leaves two subspaces of \( \mathcal{B} \) invariant: \( \mathcal{W} \), the \( d \)-dimensional subspace spanned by the basis elements \( \{e_I | I = 1, \ldots d\} \) (containing 1 and \( \tau \), and its \( d(d-1) \)-dimensional orthogonal complement \( \mathcal{W}^\perp \), spanned by the basis elements \( \{e_I | I, J = 1, \ldots d, I \neq J\} \). Thus, it uniquely decompose into the direct sum \( M'_{\otimes}(\alpha) = \mathcal{R}(\alpha) \oplus S \), where \( \mathcal{R}(\alpha) \) acts on \( \mathcal{W} \), and \( S \) acts on \( \mathcal{W}^\perp \). The components of these operators are 
\[ R_{IJ}(\alpha) = M'_{\otimes, II, JJ}(\alpha) \quad \forall I, J \]  
\( (6.23) \)
\[ S_{II, KK} = \left\{ \begin{array}{ll} M'_{\otimes, II, JJ}(\alpha) & \text{for } (IJ) = (KL), I \neq J, K \neq L \\ 0 & \text{for } (IJ) \neq (KL), I \neq J, K \neq L \end{array} \right\} \]  
\( (6.24) \)
Since the indices of $S$ are understood as pairs $IJ$ with $I \neq J$, the array $S_{IJ,KL}$ forms a diagonal $d(d-1) \times d(d-1)$ matrix. As indicated, it is independent of $\alpha$ (because the operator $P$ as defined in (6.5) acts as a projection in $\mathcal{W}$ and annihilates $\mathcal{W}^\perp$).

Some algebra shows how our measures of knowledge may be expressed in terms of these objects: Let

$$R_{IJ} = \mathcal{R}_{IJ}(0),$$

which is the $d \times d$ matrix made up be the $IIJJ$ components of (6.8) when the $\alpha P$-term is ignored, and

$$E_{IJ} = 1 \quad \forall I, J \quad (6.26)$$

reflecting the component structure of the $\alpha P$-term in (6.8). Then

$$\det \mathcal{M}' = \frac{1}{d} \det R \ Tr(R^{-1}E) \ det S \quad (6.27)$$

$$Tr(\mathcal{M}'^{-1}) = Tr(R^{-1}) - \frac{\det(\mathcal{M}'^{-1})}{Tr(R^{-1})} + \det(S^{-1}). \quad (6.28)$$

When computing these two quantities one may use the fact that they are invariant under the replacement $R \to R + cE$ for any constant $c$. The combination $\det R \times Tr(R^{-1}E)$ may likewise be written as $\sum_{I,J} (-)^{I+J} \det_{IJ} R$, where $\det_{IJ} R$ is the determinant of the matrix obtained from $R$ by deleting the $I$-the row and the $J$-th column. (We recall from linear algebra that $\det_{IJ} R = \det R_{II} (R^{-1})_{JI}$). It thus follows that $\det \mathcal{M}'$ is a polynomial expression in $R_{IJ}$.

**Comparison of efficiency for different states**

In order to compare the efficiency of an improved strategy for different states in the volume oriented approach, we note that, according to (6.6) and (6.8),

$$\mathcal{M}(\lambda \tau_1 + (1 - \lambda) \tau_2) \leq \lambda \mathcal{M}(\tau_1) + (1 - \lambda) \mathcal{M}(\tau_2) \quad 0 \leq \lambda \leq 1.$$  

Hence, as in (6.15) and (6.16), the Peierls-Bogoliubov inequality guarantees that the strategy is more efficient for a state that is less mixed, i.e.

$$\det \mathcal{M}'(\alpha, \lambda \tau_1 + (1 - \lambda) \tau_2) \leq \lambda \det \mathcal{M}'(\alpha, \tau_1) + (1 - \lambda) \det \mathcal{M}'(\alpha, \tau_2). \quad (6.29)$$

Later on, when discussing particular strategies, we will concentrate on “typical” states, i.e. the tracial state, which is maximally mixed, and states with some vanishing eigenvalues.
Strategy 1: Using mutually unbiased observables

From our result for the two-dimensional case we guess that it is a good strategy to choose one observable in the direction of \( \tau \), e.g. \( B_1 = \tau \). For simplicity, we assume that \( \tau \) is non-degenerate, its spectral projections thus being the one-dimensional operators \( e_{II} \). If \( \tau \) is degenerate, we slightly change it to some non-degenerate \( \tilde{\tau} \) and re-insert \( \tau \) in the very end of the computation. Following the spirit of Wootters and Fields [1], we seek to choose the other observables \( B_\beta (\beta \geq 2) \) such that all eigenbases are mutually unbiased. It is not known whether for arbitrary dimensions \( d \) such operators exist. However, the averaging method as developed above provides a strategy that comes close to this idea and is realizable in any dimension. It requires just one other observable, \( B_2 \), satisfying

\[
\text{Tr}(P_1 a P_2 a') = \frac{1}{d} \quad \forall a \in \text{Sp}(B_1) \text{ and } a' \in \text{Sp}(B_2).
\] (6.30)

This may also be written as

\[
P_{2a,II} = \frac{1}{d} \quad \forall a \in \text{Sp}(B_2)
\] (6.31)

and implies \( (\tau|P_{2a}) = 2/d \quad \forall a \in \text{Sp}(B_2) \). To these two observables we apply the strategy improving mechanism (6.22). If however there exists a large enough family of mutually unbiased bases, as in the explicit example given in [1], then all components \( P_{\beta a,IJ} \) of \( P_{\beta a} \) coincide up to phase factors, and we expect the strategy based on these to be equivalent to the one we will now analyze. (In the two-dimensional case, this corresponds to the fact that we can either measure in two fixed orthogonal directions – as has explicitly been worked out in the preceding section –, or alternatively in all directions orthogonal to \( \vec{u} \). In this case the averaging method does not lead to anything new).

So let us start with \( B_1 = \tau \) and \( B_2 \) satisfying (6.30). We leave \( n_1 \) and \( n_2 \) unspecified for the moment. With (6.8), the contributions to (6.22) for \( \alpha = 0 \) are as follows:

\[
n_1 Q_{II,JI}(B_1) = n_1 \sum_{a \in \text{Sp}(B_1)} \frac{P_{1a,II} P_{1a,*J}}{(\tau|P_{1a})} = n_1 \frac{1}{2} \delta_{IJ} \quad \forall I, J
\] (6.32)

\[
n_1 Q_{II,JJ}(B_1) = n_1 \sum_{a \in \text{Sp}(B_1)} \frac{|P_{1a,JI}|^2}{(\tau|P_{1a})} = 0 \quad \text{for } I \neq J
\] (6.33)
\[ n_2 Q_{II, JJ}(B_2) = n_2 \sum_{a \in \text{Sp}(B_2)} \frac{P_{2a, II} P_{2a, JJ}^*}{(\tau|P_{2a})} = \frac{n_2}{2} \quad \forall I, J \] (6.34)

\[ n_2 Q_{I, I, J}(B_2) = n_2 \sum_{a \in \text{Sp}(B_2)} \frac{|P_{2a, I, J}|^2}{(\tau|P_{2a})} = \frac{n_2}{2} \quad \text{for } I \neq J. \] (6.35)

Adding (6.32)+(6.34) and (6.33)+(6.35) gives all non-zero components of \( M'(0) \). The only nonzero components of the operators \( R \) and \( S \) as introduced in (6.23)–(6.25) are thus given by

\[ R_{I, J} = \frac{n_1}{2} \delta_{I, J} + \frac{n_2}{2} \quad \forall I, J \] (6.36)

\[ S_{I, I, J} = \frac{n_2}{2} \quad \text{for } I \neq J. \] (6.37)

Using (6.27), our final result for the volume oriented approach reads

\[ \det M' = \frac{1}{d} \left( \frac{n_1}{2} \right)^{d-1} \left( \frac{n_2}{2} \right)^{d(d-1)} \det(\tau^{-1}). \] (6.38)

For given \( n = n_1 + n_2 \), the best of all these strategies is characterized by \( n_1 n_2^d = \max \), which leads to

\[ n_1 = \frac{n}{d+1} \quad \text{and} \quad n_2 = \frac{dn}{d+1}, \] (6.39)

hence

\[ (\det M')_{\max} = d^{d^2-d-1} \left( \frac{n}{2(d+1)} \right)^{d^2-1} \det(\tau^{-1}). \] (6.40)

If \( d = 2 \), this coincides with the value (5.8) for the best two-dimensional (volume oriented) strategy. However, as we shall see, in higher dimensions there are states \( \tau \) for which one can do better. Analogously, using (6.28), we find for the distance oriented approach

\[ \text{Tr}(M'^{-1}) = \frac{2}{n_1} \left( 1 - \text{Tr}(\tau^2) \right) + \frac{2d(d-1)}{n_2}. \] (6.41)

For given \( n = n_1 + n_2 \), the best of all these strategies are characterized by

\[ n_1 = \frac{n}{1 + \sqrt{\frac{d(d-1)}{1-\text{Tr}(\tau^2)}}} \quad \text{and} \quad n_2 = \frac{n}{1 + \sqrt{\frac{1-\text{Tr}(\tau^2)}{d(d-1)}}}, \] (6.42)
hence
\[ \text{Tr}(\mathcal{M}'^{-1})_{\text{min}} = \frac{2}{n} \left( \sqrt{1 - \text{Tr}(\tau^2)} + \sqrt{d(d - 1)} \right)^2. \] (6.43)

If \( d = 2 \), this coincides with the value (5.16) for the best two-dimensional (distance oriented) strategy. Whether one can do better in higher dimensions is an open question.

Summarizing, the strategies specified by (6.39) and (6.42) are in a sense the natural generalizations from the two-dimensional case, their effectiveness being quantified by (6.40) and (6.43).

**Strategy 2: Using matrix units**

We will now – for even dimensions – construct a different strategy that sometimes works better in the volume oriented approach. From the two-dimensional situation we have learned the following: The uncertainties (in both the volume and the distance oriented approach) are smaller when the unknown state is less mixed. As in the strategy constructed above, we choose one observable, \( B_1 \), coinciding with \( \tau \). The other observables should give as much new information as possible, therefore should be sufficiently independent of \( \tau \). They are maximally independent if they are mutually unbiased. However, then the uncertainties tend to be large. Therefore two effects are competing, and we have observed that in two dimensions the independence is the dominating effect. In higher dimensions, a convenient basis of \( \mathcal{B} \) is given by the matrix units (6.1), constructed out of an eigenbasis of \( \tau \). Since these operators are not positive (not even hermitian) and therefore do not correspond to observables, we resort to the \( d(d - 1) \) projections defined by
\[ P_{IJ}^\pm = \frac{1}{2} (e_{II} \pm e_{IJ} \pm e_{JI} + e_{JJ}). \] (6.44)

Our goal is to construct the rest of our observables out of these operators. As before, we understand that the average procedure (6.22) has been performed. In effect this just means to take into account only the components of \( \mathcal{M}_{\phi_{IJ},KL}(0) \) relevant for \( R_{IJ} \) and \( S_{IJ,JI} \) as defined in (6.23)–(6.25). Any \( P_{KL}^\pm (K < L) \) appearing as spectral projection of an observable \( B_\beta \) gives the contributions
\[ n_\beta \frac{P_{KL,II}^\pm P_{KL,JJ}^\pm}{(\tau|P_{KL}^\pm)} = \frac{n_\beta}{4} \frac{(\delta_{IK} + \delta_{IL})(\delta_{JK} + \delta_{JL})}{\tau_{KK} + \tau_{LL}} \quad \forall I, J \] \[ n_\beta \frac{|P_{KL,II}^\pm|^2}{(\tau|P_{KL}^\pm)} = \frac{n_\beta}{4} \frac{\delta_{IK} \delta_{IL} + \delta_{IK} \delta_{JL}}{\tau_{KK} + \tau_{LL}} \quad \text{for } I \neq J \] (6.45) (6.46)
to $R_{I,J}$ and $S_{I,I,J}$, respectively. These expressions have to be summed up for all projectors involved. The contributions from $B_1$ are identical with (6.32)–(6.33).

Let us now show how the projections (6.44) may be used to define suitable observables. The idea is to group these operators into $d-1$ subfamilies, each containing $d$ elements, in order to construct $d-1$ observables in addition to $B_1$. We will restrict ourselves to even $d$ and define $B_2$ to have the spectral projections (the eigenvalues being irrelevant as long as each observable is non-degenerate)

$$P_{12}^±, P_{12}^−, P_{34}^±, \ldots P_{(d-1),d}^±.$$

This may be abbreviated in terms of the partition

$$B_2 \leftrightarrow (1,2)(3,4)\ldots(d-1,d)$$

of $(1,2,\ldots,d)$. The remaining observables are obtained by appropriately permuting certain numbers in the above partition, such that any pair never occurs twice. This is possible in any even dimension and can best be explained in an example: For illustration we choose $d=6$ and define

$$B_2 \leftrightarrow (1,2)(3,4)(5,6)$$

$$B_3 \leftrightarrow (1,3)(2,5)(4,6)$$

$$B_4 \leftrightarrow (1,5)(3,6)(2,4)$$

$$B_5 \leftrightarrow (1,6)(5,4)(3,2)$$

$$B_6 \leftrightarrow (1,4)(6,2)(3,5)$$

The underlying general procedure is the following: One number in every pair is moving to the right, one to the left as long as it is possible, then it is reflected. In this way every number corresponds to a line, and every line crosses every other line exactly once. For $d > 4$ there are other possible permutation schemes (which should all be taken into account when the best of these strategies is to be determined). A strategy is fixed by giving any observable $B_β (β = 1,\ldots,d)$ a weight $n_β$, the number of measurements reserved for the family $B_β(φ)$, such that $\sum_{β=1}^d n_β = n$.

In order to write down the operators $R$ and $S$ for this type of strategy, we note that, for given $K, L (K \neq L)$, either the pair $P_{KL}^±$ or the pair $P_{LK}^±$ occurs in some
Let us denote this \( \beta \) by \( \beta(K, L) \). Using this notation, we sum up (6.45) and (6.32) for \( R \), (6.46) and (6.33) for \( S \), to obtain

\[
R_{IJ} = \delta_{IJ} \left( \frac{n_1}{2\tau_{II}} + \sum_{K \neq I} \frac{n_{\beta(I,K)}}{2(\tau_{II} + \tau_{KK})} \right) + (1 - \delta_{IJ}) \frac{n_{\beta(I,J)}}{2(\tau_{II} + \tau_{JJ})} \tag{6.50}
\]

\[
S_{I,I,J} = \frac{n_{\beta(I,J)}}{2(\tau_{II} + \tau_{JJ})} \quad \text{for } I \neq J. \tag{6.51}
\]

The explicit evaluation of (6.27) and (6.28) for a general strategy of this type and comparison with our previous results (6.40) and (6.43) is not an easy task. We will therefore confine ourselves to a family of examples: Let \( d \geq 4 \), \( \tau_{11} = \tau_{22} = a/2 \) and \( \tau_{33} = \ldots = \tau_{dd} = (1 - a)/(d - 2) \), and set \( n_{\beta} = n' \) for all \( \beta = 2 \ldots d \) (i.e. \( n_{\beta(I,J)} = n' \) for all \( I \neq J \)). For small \( a \), the combination \((\tau_{11} + \tau_{22})^{-1}\) is large. This blows up the determinant of \( \mathcal{M} \): We find \( R_{11} = R_{22} = n_1/a + O(1) \) and \( R_{12} = R_{21} = S_{1212} = S_{2121} = n'/2a + O(1) \), whereas all other components are finite for \( a \to 0 \). The application of (6.27) to (6.50)–(6.51) exhibits the behaviour

\[
\det \mathcal{M}' \sim O(a^{-d^2}) \quad \text{for small } a. \tag{6.52}
\]

This may be compared with (6.40) which – for the same \( \tau \) – diverges only as \( O(a^{-2}) \). Hence, for given even dimension \( d \geq 4 \), there is always an unknown state \( \tau \) (defined by sufficiently small \( a \)) such that a strategy of type 2 is better than strategy 1 in the volume oriented approach. For the distance oriented approach, there is no such difference in the scaling behaviour for \( a \to 0 \).

For \( a = 2/d \), we obtain the tracial state \( \tau = d^{-1}1 \), i.e. \( \tau_{II} = d^{-1} \) for all \( I \). In this case we can be more explicit, and we obtain

\[
\det \mathcal{M}' = \left( \frac{d}{4} \right)^{d^2 - 1} \left[ 2n_1 + n'(d - 2) \right]^{d} \tag{6.53}
\]

\[
\text{Tr}(\mathcal{M}'^{-1}) = 4(d - 1) \left( \frac{1}{2n_1 + n'(d - 2)} + \frac{1}{n'} \right). \tag{6.54}
\]

Interestingly, if \( d \geq 4 \), both expressions become optimized if \( n_1 = 0 \), i.e. \( n' = n/(d - 1) \). Hence, the best values for this class of strategies for the tracial state are given by

\[
(\det \mathcal{M}')_{\text{max}} = \left( \frac{d}{4} \right)^{d^2 - 1} \left( d - 2 \right) \left( \frac{n}{d - 1} \right)^{d + 1} \tag{6.55}
\]
\[
\text{Tr}(\mathcal{M}'^{-1})_{\text{min}} = \frac{4(d-1)^4}{n(d-2)d^4}. \quad (6.56)
\]

The volume oriented strategy (6.55) gets beaten by (6.40), because – for the tracial state – (6.40) ≥ (6.55) for all \( d \). Asymptotically for large \( d \), (6.40) exceeds (6.55) by a factor of leading order \( 2d^2 \). Similarly, the distance oriented strategy (6.56) is worse than (6.43), because, for large \( d \), (6.56) is twice as large as (6.43) for the tracial state.

It is easy to show that the last feature remains true for general states if \( d \geq 6 \):

Using the estimates

\[
\text{Tr}(S^{-1}) = \sum_{I \neq J} S^{-1}_{I,J,J} = \sum_{I \neq J} \frac{2(\tau_{II} + \tau_{JJ})}{n_{\beta(I,J)}} \geq \sum_{\beta} \frac{2}{n_{\beta}} \geq \frac{4(d-1)^2}{n - n_1} \quad (6.57)
\]

\[
\text{Tr}(R^{-1}) - \frac{\text{Tr}(R^{-1}ER^{-1})}{\text{Tr}(R^{-1}E)} \geq 0 \quad (6.58)
\]

together with (6.28), we find

\[
\text{Tr}(\mathcal{M}'^{-1}) \geq \frac{4(d-1)^2}{n}. \quad (6.59)
\]

From this it follows that also for general states in \( d \geq 6 \) our strategy of type 2 cannot beat (6.43).

Summarizing, for even dimensions \( \geq 4 \), there are states \( \tau \) for which the strategy (6.40) based on mutually unbiased observables is not optimal when evaluated in the volume oriented approach. On the other hand, in the distance oriented approach, we cannot offer a strategy better than (6.43).

**Remarks on infinite dimensions**

The results achieved in this paper suggest that the number of measurements necessary in order to arrive at an estimate of the unknown state \( \tau \) with an uncertainty of the order \( \epsilon \) increases like \( d^2 \) with increasing dimension \( d \) of the Hilbert space \( \mathcal{H} \).

This may be seen in both approaches we discussed: Identifying \( \epsilon^2 \) with \( \text{Tr}(\mathcal{M}^{-1}) \) in the distance oriented approach, (6.43) implies \( \epsilon^2 \approx 2d^2/n \), hence \( n \sim (d/\epsilon)^2 \). The
analogous situation for the volume oriented approach is roughly modeled by identifying \((\det \mathcal{M})^{-1/2}\) with the volume of a sphere of radius \(\epsilon\) in \((d^2 - 1)\)-dimensional Euclidean space. Using Stirling’s formula, the latter is for large \(d\) given by

\[
\mathcal{V}_d \approx \frac{\epsilon^{d^2-1}}{\sqrt{(d^2 - 1)\pi}} \left( \frac{2e\pi}{d^2 - 1} \right)^{(d^2-1)/2}.
\]  

With (6.40) – the strategy based on mutually unbiased observables – and fixed \(\det(\tau^{-1})\), this gives \(n \sim (d/\epsilon)^2\) as in the distance oriented approach. This behaviour is confirmed by the strategies of type 2 (using matrix units) which were found to be better for certain states. Since we need an additional number of measurements to get a first rough estimate of \(\tau\), the formula \(n \sim (d/\epsilon)^2\) is to be understood as the leading asymptotic behaviour of \(n\) as \(\epsilon\) approaches 0.

If this behaviour is true for the best strategies possible, it has dramatic consequences for the infinite dimensional case: At first glance, it would altogether be impossible to determine \(\tau\) with some (given) uncertainty \(\epsilon\). However, in infinite dimensions we may decompose the Hilbert space as \(\mathcal{H} = P_d(\mathcal{H}) \oplus P_d(\mathcal{H})^\perp\), where \(P_d\) is some finite \((d-)\)dimensional hermitian projection, and measure \(P_d\) in a number of copies of our quantum system. Starting with \(d = 1\), we choose a one-dimensional hermitian projection \(P_1\). Whenever the measurement outcome is 0, i.e. corresponds to \(P_d(\mathcal{H})^\perp\), we redefine \(d_{\text{new}} = d + 1\), choose some new decomposition such that \(P_{d_{\text{new}}} \geq P_d\), and proceed analogously. During this process, the probability for 0 to occur in a further measurement, given by \(1 - \text{Tr}(\tau P_d)\), drops down to zero as \(d\) increases. In other words, the measurement data become increasingly consistent with the expectation that \(\tau\) is a density matrix in \(P_d(\mathcal{H})\). If \(\rho_{\text{ex}}\) is the expected state, the uncertainty \(\epsilon\) about \(\tau\) is given by \(\epsilon^2 \approx \text{Tr}((\tau - \rho_{\text{ex}})^2)\). In terms of an appropriate block matrix notation we have

\[
\rho_{\text{ex}} = \begin{pmatrix} \rho_d & 0 \\ 0 & 0 \end{pmatrix}, \quad \tau = \begin{pmatrix} \tau_d & \nu_d \\ \nu_d^\dagger & \tau_\infty \end{pmatrix},
\]

so that \(\text{Tr}((\tau - \rho_{\text{ex}})^2) = \text{Tr}((\tau_d - \rho_d)^2) + 2 \text{Tr}(\nu_d\nu_d^\dagger) + \text{Tr}(\tau_\infty^2)\). For given \(\epsilon_0 > 0\), there is a (finite) dimension \(d_{\text{eff}}\) and a (finite) number \(n_0\) of measurements necessary to make sure that \(2 \text{Tr}(\nu_{d_{\text{eff}}}\nu_{d_{\text{eff}}}^\dagger) + \text{Tr}(\tau_\infty^2) \lesssim \epsilon_0^2\). The numbers \(d_{\text{eff}}\) and \(n_0\) will depend on \(\tau\) and on the sequence of projections \(P_1, P_2, \ldots\) chosen. Once having reached this point, we proceed as if \(\tau\) acts entirely in the subspace \(P_{d_{\text{eff}}}(\mathcal{H})\). (Technically, we measure observables of the type \(A \oplus (1 - P_{d_{\text{eff}}}^\perp)\), where \(A\) acts in \(P_{d_{\text{eff}}}(\mathcal{H})\), and ignore further
outcomes that belong to the remaining infinite dimensional subspace $P_{d_{\text{eff}}} (\mathcal{H})^\perp$.

Next, given $\epsilon_1$, we need a further number $n_1 \sim (d_{\text{eff}}/\epsilon_1)^2$ of measurements to arrive at a final estimate $\rho_{\text{fin}}$ in $P_{d_{\text{eff}}} (\mathcal{H})$ such that $\text{Tr}((\tau_{d_{\text{eff}}} - \rho_{\text{fin}})^2) \lesssim \epsilon_1^2$. Hence, after $n = n_0 + n_1$ measurements, the total uncertainty is of the order $\epsilon = (\epsilon_0^2 + \epsilon_1^2)^{1/2}$.

This procedure enables one to determine an unknown state to any desired degree of security even if it lives in an infinite dimensional Hilbert space. (This is of course not an optimal strategy. A more efficient method is e.g. to combine the two parts of the procedure and to measure observables of the type $A \oplus (1 - P_d)$ from the outset).

The apparent contradiction of this result with the behaviour $n \sim (d/\epsilon)^2$ in the case of large but finite dimension $d$ is clarified by noting that the number $n_0$ may be very large: Suppose some sequence of projections $P_{d+1} = P_d + |e_{d+1}\rangle\langle e_{d+1}|$ has been fixed ($e_I$ denoting an orthonormal basis of $\mathcal{H}$, the starting point being $P_1 = |e_1\rangle\langle e_1|$), and suppose that $\tau = |e_D\rangle\langle e_D|$ for some $D$ (that may be very large). In this case it takes $D$ measurements until a non-zero outcome is possible. Similar scenarios are possible for any $\tau$: Given an arbitrary number $N$, then (with some portion of bad luck) it is always possible to adjust the sequence of projections such that $n_0 > N$. Hence, there exists no general upper bound for $n_0$ (and thus for $n$). This feature is not present in the finite dimensional case. The behaviour $n \to \infty$ as obtained by letting $d \to \infty$ in the formula $n \sim (d/\epsilon)^2$ must be understood in this sense.

A problem still persists with our approach. It stems from the fact that we have invoked a Gaussian approximation. For finite dimension $d$ we infer from (2.15) and (2.22) that this approximation is reliable if $\epsilon \parallel \tau^{-1} \parallel \ll 1$. In other words: if $\epsilon$ is chosen too large, our formalism will fail to reproduce the unknown state with the promised accuracy. As a consequence, we must have $n \gg d^2 \parallel \tau^{-1} \parallel$, which means that a smaller number of measurements will not lead to a reasonable result. This introduces an additional dependence on the dimension into the state determination problem: Since $\parallel \tau^{-1} \parallel \geq d$, we have $\epsilon \ll d^{-1}$ and $n \gg d^3$. However, in large dimensions, typical density matrices tend to have even larger $\parallel \tau^{-1} \parallel$. In the infinite dimensional case, $\parallel \tau^{-1} \parallel$ is no longer finite. Even when reducing the problem to an effectively finite dimensional one, as sketched above, we can expect the density matrix $\tau_{d_{\text{eff}}}$ to have a very large (if not infinite) value of $\parallel \tau_{d_{\text{eff}}}^{-1} \parallel$. This in turn requires the choice of a correspondingly small $\epsilon$ and blows up $n$. A partial cure of this dilemma is to modify the determination of $P_{d_{\text{eff}}} (\mathcal{H})$ so as to statistically test any redefinition $d_{\text{new}} = d + 1$ whether a large enough portion of $\tau$ is gained, and
undo it otherwise. Thus, the small eigenvalues of $\tau$ may be kept in $P_{\text{det}}(\mathcal{H})^\perp$, and only the large ones are taken into account. In effect, we expect such a procedure to reduce the number of measurements necessary.

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