

Guessing Quantum Ensemble Using Laplace Principle

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January 23, 2009

Abstract

For a mixed quantum state with density matrix ρ there are infinitely many ensembles of pure quantum states, which average to ρ . Starting from Laplace principle of insufficient reason (not to give *a priori* preference to any particular state), we derive a ‘natural’ distribution of pure states averaging to ρ , which is ‘more spread’ than all the others.

1 Introduction

In classical situation an unknown probability distribution can be estimated by collecting statistics. This is not the case in quantum mechanics when we need to estimate a distribution of pure quantum states. All we can do is to estimate the density matrix ρ of appropriate mixed quantum state. Although, there are infinitely many distributions of pure quantum states which average to the density matrix ρ . That is why in order to estimate the distribution, that is, the ensemble of pure quantum states, some *a priori* assumption about this distribution is required. Which one?

It was Laplace who introduced the formula of classical probability [1]

$$P = \frac{m}{n}$$

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where n stands for the total number of outcomes and m is the number of favorable ones. This formula is not *ad hoc* introduced. Rather, it based on the *principle of insufficient reason*:

if there is no reason to prefer one outcome of an experiment with respect to another one, all outcomes are treated equally probable.

According to Laplace, if we are given a completely unknown distribution and we need to estimate it, we assume it to be just uniform. But what should we do if we have an additional information about the distribution? Can we still use Laplace principle?

2 A classical example: exploring biased die

Suppose we play with die whose properties are not known. If we are asked what is the probability of a certain face to appear, we intuitively (but in fact according to Laplace) answer: ‘there are 6 faces, none of them is preferred, hence any face appears with the same probability $1/6$ ’.

We roll N identical dice and, as a result of this experiment, we learn the mean value, denote it M , of the number of shown points. This is an information about the die, how it affects our estimation? In this case the hypothesis of the equality of all *faces* may no longer be compatible with initial hypothesis that all faces are the same (indeed, one would scarcely believe a die showing $M = 5$ points at average to be symmetric). So, the Laplace principle is not applicable, at least in its direct form.

Consider it in a more general setting. Suppose we have N identical dice with K faces each. Each face k is labeled by a value A_k and the die might be ‘biased’, that is, the probability of k -th face to appear is an unknown number p_k . N such identical dice are rolled, and the average value of the number appeared turns out to be M . What can we now say about p_k ?

This average value M can be obtained when we have n_1 times face $1, \dots, n_K$ times face K , with the values $\{n_1, \dots, n_K\}$ satisfying the equations

$$\begin{aligned} n_1 + \dots + n_K &= N \\ A_1 \cdot n_1 + \dots + A_K \cdot n_K &= M \cdot N \end{aligned} \tag{1}$$

When the number N is large, we may treat

$$p_k = \frac{n_k}{N} \tag{2}$$

The solution of (1) with respect to $\{n_1, \dots, n_K\}$ is, however, far from being unique. Meanwhile, the solutions do not possess equal rights: each particular solution $\{n_1, \dots, n_K\}$, according to Bernoulli formula, has *a priori* probability

$$P(n_1, \dots, n_K) = \frac{N!}{n_1! \dots n_K!} p_1^{n_1} \dots p_K^{n_K}$$

Maximizing the value of the probability $P(n_1, \dots, n_K)$, among the solutions $\{n_1, \dots, n_K\}$, satisfying (1) we find one, which has greatest probability, therefore we . Using Stirling formula we get (see, e.g. [2] for details):

$$\log P(n_1, \dots, n_K) \sim N \cdot \left(-\frac{n_1}{N} \log \frac{n_1}{N} - \dots - \frac{n_K}{N} \log \frac{n_K}{N} \right) \quad (3)$$

The above formula is the Shannon entropy

$$\frac{1}{N} \log P(n_1, \dots, n_K) \sim -p_1 \log p_1 - \dots - p_K \log p_K \quad (4)$$

and the maximum of $\log P(n_1, \dots, n_K)$ is attained at

$$p_k = \frac{n_k}{N} \sim \frac{e^{-\beta A_k}}{Z} \quad (5)$$

where Z is the normalizing factor

$$Z = \sum_k e^{-\beta A_k} \quad (6)$$

and β is a ‘temperature parameter’, obtained by solving (1) in explicit form

$$\frac{A_1 e^{-\beta A_1} + \dots + A_K e^{-\beta A_K}}{e^{-\beta A_1} + \dots + e^{-\beta A_K}} = \frac{M}{N} \quad (7)$$

with respect to β . This gives us definite values of p_1, \dots, p_K ¹.

As an illustration, consider a usual die, that is $K = 6$, $A_1 = 1, \dots, A_6 = 6$. Begin with a symmetric case $M = (1 + 2 + \dots + 6)/6 = 3.5$. The solution of (7) is $\beta = 0$, which means that the Laplace principle still works and this particular value of M gives no preference to any state, therefore the null hypothesis (the uniform distribution $p_j = 1/6$) should not be rejected.

¹Recall that we know only M and we wish to infer from this knowledge the ‘natural’ values of p_1, \dots, p_K .

If the die is ‘*biased*’, we obtain a different value of M , say, $M = 2.5$. In this case the Laplace principle should be expanded: namely, we search the distribution maximizing the entropy $H = -\sum p_j \log p_j$. In our particular case this gives the following answer:

$$p_j = \frac{e^{-\beta j}}{Z} \tag{8}$$

Solving numerically (7) for $M = 2.5$ gives us $\beta = 0.3710$, that is

$$\{p_1, p_2, \dots, p_6\} = \{0.3476, 0.2396, 0.1654, 0.1143, 0.0788, 0.0543\}$$

The main message of this section is the following. We provide a completely classical example where we have *no knowledge* about the input state (distribution) but we *need* to tell something about it. A principle is described to choose a concrete distribution on the basis of a given small amount of knowledge.

3 Continuous ensembles

Why the idea to maximize the entropy H is a development of Laplace idea of symmetry and non-preference? For any given average value we consider all possible distributions which yield this average value. Then we take such distributions which are typical, that is, which mostly occur in all possible configurations [4]. The preference is given to what occur with maximal number of combinations, expressed by the statistical weight

$$P = \frac{N!}{\prod_j n_j} \sim N \cdot \left(-\sum_j \frac{n_j}{N} \log \frac{n_j}{N} \right)$$

where N is the total number of trials and n_j is number of occurrence of j -th face (j -th outcome, more generally).

Now let us develop a similar construction, but passing from numbers to operators, that is, the mean value is now an operator rather than a number M in (1). The restriction (1) becomes of matrix form. The consequence of this is that the value of the parameter β —appropriate Lagrange multiple—becomes matrix as well.

Let $\mathcal{H} = \mathbf{C}^n$ be an n -dimensional Hermitian space, let ρ be a density matrix in \mathcal{H} . There are infinitely many ensembles whose average density

matrix is ρ . Among them we would like to emphasize a ‘natural’ one. First suppose this ensemble to be finite and, like in previous section, in order to find a natural ensemble, maximize its mixing entropy. The result is the following: given any arbitrary large number E , we can always find an ensemble of 2^E pure states which averages to ρ and whose mixing entropy is E : this is a uniform ensemble [3]. So, there is no limit for mixing entropy for finite ensembles. As a result, we pass to continuous ensembles with the distribution density expressed by a function $\mu(\phi)$ where ϕ ranges over all unit vectors² in \mathcal{H} .

The set of all self-adjoint operators in $\mathcal{H} = \mathbf{C}^n$ has a natural structure of a real space \mathbf{R}^{2n} , in which the set of all density matrices is a hypersurface, which is the zero surface $T = 0$ of the affine functional $T = \text{Tr } X - 1$. The density operator of a continuous ensemble associated with the measure $\mu(\phi)$ on the set $\mathbf{C}B_n$ of unit vectors in \mathcal{H} is calculated as the following (matrix) integral

$$\rho = \int_{\phi \in \mathbf{C}B_n} \mu(\phi) |\phi\rangle\langle\phi| \, d\psi \quad (9)$$

where $|\phi\rangle\langle\phi|$ is the projector onto the vector $\langle\phi|$ and $d\psi$ is the above mentioned normalized measure on $\mathbf{C}B_n$, that is, $\int_{\phi \in \mathbf{C}B_n} d\psi = 1$. Effectively,

the operator integral ρ in (9) can be calculated by its matrix elements. In any fixed basis $\{|\mathbf{e}_i\rangle\}$ in \mathcal{H} , each its matrix element $\rho_{ij} = \langle\mathbf{e}_i|\rho|\mathbf{e}_j\rangle$ is the following numerical integral:

$$\rho_{ij} = \langle\mathbf{e}_i|\rho|\mathbf{e}_j\rangle = \int_{\phi \in \mathbf{C}B_n} \mu(\phi) \langle\mathbf{e}_i|\phi\rangle \langle\phi|\mathbf{e}_j\rangle \, d\psi \quad (10)$$

Kullback–Leibler distance. We quantify the state preparation efforts by the difference between the entropy of uniform distribution (that is, our null

²Pure states form a projective space rather than the unit sphere in \mathcal{H} . On the other hand, one may integrate over any probabilistic space. Usually distributions of pure states over the spectrum of observables are studied, sometimes probability distributions on the projective spaces are considered [5]. In this paper for technical reasons we prefer to represent ensembles of pure states by measures on unit vectors in \mathcal{H} . We use the Umegaki measure on $\mathbf{C}B_n$ —the uniform measure with respect to the action of $U(n)$ normalized so that $\int_{\mathbf{C}B_n} d\psi = 1$.

hypothesis) and the entropy of the ensemble³ in question. This is equal to Kullback-Leibler distance [2]

$$S(\mu\|\mu_0) = \int \mu(x) \ln \frac{\mu(x)}{\mu_0(x)} dx$$

between the distribution $\mu(x)$ and the uniform distribution $\mu_0(x)$ with constant density, normalize the counting measure dx on the probability space so that $\mu_0 = 1$. This distance is the average likelihood ratio, on which the choice of statistical hypothesis is based. Then, in order to minimize the Type I error we have to choose a hypothesis with the smallest average likelihood ratio.

Maximizing the entropy. The problem reduces to the following. For given density matrix ρ find a continuous ensemble μ having minimal differential entropy:

$$S(\mu) = \int \mu(x) \ln \mu(x) dx \rightarrow \min, \quad \int |\psi\rangle\langle\psi| \mu(\psi) d\psi = \rho \quad (11)$$

where $d\psi$ is the unitary invariant measure on pure states normalized to integrate to unity. When there is no constraints in (11), the answer is straightforward—the minimum (equal to zero) is attained on uniform distribution—this situation is quite similar to the symmetric classical case considered in section 2. To solve the problem with constraints, we use the Lagrange multiples method [7]. The appropriate Lagrange function reads:

$$\mathcal{L}(\mu) = S(\mu) - \text{Tr} \Lambda \left(\int |\psi\rangle\langle\psi| \mu(\psi) d\psi - \rho \right)$$

where the Lagrange multiple Λ is a matrix since the constraints in (11) are of matrix character. Substituting the expression for $S(\mu)$ and making the derivative of \mathcal{L} over μ zero, we get

$$\mu(\psi) = \frac{e^{-\text{Tr} B |\psi\rangle\langle\psi|}}{Z(B)} \quad (12)$$

where B is the optimal value of the Lagrange multiple Λ which we derive from the constraint (11) and the normalizing multiple

$$Z(B) = \int e^{-\text{Tr} B |\psi\rangle\langle\psi|} d\psi \quad (13)$$

³We are speaking here of *mixing entropy* [6] of the ensemble rather than about von Neumann entropy of its density matrix.

is the partition function for (12).

4 Conclusions

In Classical Mechanics, there is a unique correspondence between mixed states and ensembles of pure states. This is no longer the case in quantum mechanics: if we are given a state described by a density matrix ρ , there are infinitely many ensembles of pure quantum states, which average to ρ . In our paper we consider quantum systems with finite-dimensional state space $\mathcal{H} = \mathbf{C}^n$. An ensemble of pure states is understood in a mostly general sense as a certain distribution of pure states in \mathcal{H} , rather than a finite weighted sum.

Contrary to conventional approach, we exploit continuous distributions of state vectors (but still in finite dimensions \mathbf{C}^n). The task we tackle is the following, Suppose we are given a quantum state with a density matrix ρ , and this is all we know about the preparation procedure. In this setting, what could we say about the ensemble, which gave rise to ρ ? In order to answer this question, we use standard statistical approach: among all ensembles averaging to ρ we choose the one which is more spread than the others. What means more spread?

We consider all ensembles averaging to ρ and, according to Laplace, give no preference to any of them. As stated above, by ensemble we mean a distribution and as a zero hypothesis we take it to be uniform — no knowledge, no preference. However, when $\rho \neq 1$, this hypothesis is not compatible with our knowledge that the average quantum state is ρ . In order to comply with Laplace principle [4] we choose the distribution of pure states which

- averages to the state ρ
- has the greatest differential entropy

The resulting distribution has the form (11): $S(\mu) = \int \mu(\phi) \ln \mu(\phi) d\phi \rightarrow \min$. So, summarizing our result

if we have a source of particles whose average quantum state is ρ , and this is the only information about the source of these particles, we have to state that they are prepared as follows: pure states are emitted with probability density

$$\int e^{-\langle \phi | B | \phi \rangle} |\phi\rangle\langle\phi| d\phi$$

Acknowledgements. The second author acknowledges the hospitality of organizers and particularly Jarosław Pykacz. The work was carried out under the auspices of the research grant RFFI 0706-00119.

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The existence of lazy ensembles

Let ρ be a nondegenerate density operator, that is, $0 < \lambda_1 \leq \dots \leq \lambda_n$, where $\{\lambda_j\}$ are the eigenvalues of the operator ρ . We are going to prove that for any such ρ there exists an operator Y such that

$$\int e^{\langle \phi | Y | \phi \rangle} |\phi\rangle\langle\phi| \, d\phi = \rho \quad (14)$$

From now on all the integrals are taken over the unit sphere in \mathbf{C}^n (if otherwise not written explicitly), and $d\phi$ is the invariant measure on it induced by Lebesgue measure in \mathbf{R}^{2n} . Fix a density matrix ρ and consider the scalar-valued function

$$Z_\infty = \int e^{\langle \phi | Y | \phi \rangle} \, d\phi - \text{Tr}(Y\rho) \quad (15)$$

and search for its minimum. If the minimum exists, then the necessary condition for it is vanishing of all partial derivatives

$$\frac{\partial Z_\infty}{\partial Y} = 0$$

which is equivalent to (14), that is, if the minimal value of (15) exists, then Y , at which it is attained, yields the solution for (14). So, we only have to prove the existence of the minimum of the function Z_∞ (15). Consider a sequence of functions Z_M parameterized by integer M :

$$Z_M(Y) = \int \left(1 + \frac{\langle \phi | Y | \phi \rangle}{2M} \right)^{2M} \, d\phi - \text{Tr}(Y\rho)$$

for them, the existence of minimum is straightforward since Z_M is a mixture of positive concave functions. That means, the (operator) equation

$$\int \left(1 + \frac{\langle \phi | Y | \phi \rangle}{2M} \right)^{2M-1} |\phi\rangle\langle\phi| \, d\phi = \rho \quad (16)$$

always has a solution Y (this Y depends on M). Let us evaluate the eigenvalues of Y , denote them $y_1 \leq \dots \leq y_n$ appropriately ordered. That is, for any ϕ

$$y_1 \leq \langle \phi | Y | \phi \rangle \leq y_n$$

hence

$$\begin{aligned}
& \left(1 + \frac{y_1}{2M}\right)^{2M-1} \int |\phi\rangle\langle\phi| \, d\phi \leq \\
& \leq \int \left(1 + \frac{\langle\phi|Y|\phi\rangle}{2M}\right)^{2M-1} |\phi\rangle\langle\phi| \, d\phi \leq \\
& \leq \left(1 + \frac{y_n}{2M}\right)^{2M-1} \int |\phi\rangle\langle\phi| \, d\phi
\end{aligned}$$

taking the trace we get

$$\left(1 + \frac{y_1}{2M}\right)^{2M-1} \leq \text{Tr } \rho \leq \left(1 + \frac{y_n}{2M}\right)^{2M-1}$$

Since we are dealing with a density operator ρ , its trace equals 1, therefore

$$y_1 \leq 0 \leq y_n \tag{17}$$

Now let us evaluate the difference $y_n - y_1$ between the greatest and the least eigenvalues of Y from (16). Let $|\mathbf{e}_j\rangle$ be an eigenvector of ρ associated with the eigenvalue λ_j , then (16) reads:

$$\lambda_j = \int_{t_1+\dots+t_{n-1}\leq 1} \left(1 + \frac{y_1 t_1 + \dots + y_{n-1} t_{n-1} + y_n(1 - t_1 - \dots - t_{n-1})}{2M}\right)^{2M-1} t_j \, dt_1 \cdots dt_{n-1}$$

therefore $(y_n - y_1)\lambda_1 =$

$$\begin{aligned}
& = \int_{t_2+\dots+t_{n-1}\leq 1} dt_2 \cdots dt_{n-1} \int_{t_1=0}^{1-t_2-\dots-t_{n-1}} \left(1 + \frac{(y_1 - y_n)t_1 + y_n + \sum_{k=2}^{n-1}(y_k - y_n)t_k}{2M}\right)^{2M-1} t_1 (y_n - y_1) \, dt_1 = \\
& = - \int_{t_2+\dots+t_{n-1}\leq 1} dt_2 \cdots dt_{n-1} \left[\left(1 + \frac{(y_1 - y_n)t_1 + y_n + \sum_{k=2}^{n-1}(y_k - y_n)t_k}{2M}\right)^{2M} t_1 \right]_{t_1=0}^{1-t_2-\dots-t_{n-1}} - \\
& \quad - \int_{t_1=0}^{1-t_2-\dots-t_{n-1}} \left(1 + \frac{(y_1 - y_n)t_1 + y_n + \sum_{k=2}^{n-1}(y_k - y_n)t_k}{2M}\right)^{2M} dt_1 \Big]
\end{aligned}$$

The first summand in the above expression is minus an integral of a non-negative function, the second is the following integral over the unit sphere

$$\int_{t_1+\dots+t_{n-1}\leq 1} \left(1 + \frac{(y_1 - y_n)t_1 + y_n + \sum_{k=2}^{n-1} (y_k - y_n)t_k}{2M} \right)^{2M} dt_1 dt_2 \dots dt_{n-1}$$

denote it by K and rewrite in a more familiar form:

$$K = \int_{t_1+\dots+t_n=1} \left(1 + \frac{\sum_{k=1}^n y_k t_k}{2M} \right)^{2M} dt_1 dt_2 \dots dt_{n-1} = \int \left(1 + \frac{\langle \phi | Y | \phi \rangle}{2M} \right)^{2M} d\phi$$

then

$$(y_n - y_1)\lambda_1 \leq K \tag{18}$$

Using (16) and taking into account that $\left(1 + \frac{\langle \phi | Y | \phi \rangle}{2M} \right)^{2M-1} \left(1 + \frac{\langle \phi | Y | \phi \rangle}{2M} \right)$, we have

$$\begin{aligned} K &= \text{Tr } \rho + \int \left(1 + \frac{\langle \phi | Y | \phi \rangle}{2M} \right)^{2M-1} \frac{\langle \phi | Y | \phi \rangle}{2M} d\phi \leq \\ &\leq \text{Tr } \rho + \text{Tr } \rho \frac{y_n - y_1}{2M} = 1 + \frac{y_n - y_1}{2M} \end{aligned}$$

since $y_n - y_1 \leq \langle \phi | Y | \phi \rangle$. Therefore

$$(y_n - y_1)\lambda_1 \leq K \leq 1 + \frac{y_n - y_1}{2M}$$

so $(y_n - y_1) \left(\lambda_1 - \frac{1}{2M} \right) \leq 1$. That is, for any $M > \lambda_1$ we have $\lambda_1 - \frac{1}{2M} \geq \frac{\lambda_1}{2}$, therefore

$$(y_n - y_1) \leq 2/\lambda_1 \tag{19}$$

This means that for sufficiently big M the solutions $\{y_1, \dots, y_n\}$ of (14) remain in the compact set:

$$\begin{cases} y_1 \leq 0 \leq y_n \\ (y_n - y_1) \leq 2/\lambda_1 \end{cases}$$

Therefore the limit of the solutions exist which means that for any nondegenerate density operator ρ there always exists the appropriate lazy ensemble

$$\int e^{-\langle \phi | B | \phi \rangle} |\phi\rangle\langle\phi| d\phi = \rho$$