‘Lazy’ quantum ensembles

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Abstract

We compare different strategies aimed to prepare an ensemble with a given density matrix \( \rho \). Preparing the ensemble of eigenstates of \( \rho \) with appropriate probabilities can be treated as ‘generous’ strategy: it provides maximal accessible information about the state. Another extremity is the so-called ‘Scrooge’ ensemble, which is mostly stingy to share the information. We introduce ‘lazy’ ensembles which require minimal efforts to prepare the density matrix by selecting pure states with respect to completely random choice.

We consider two parties, Alice and Bob, playing a kind of game. Bob wishes to guess which pure state is prepared by Alice. His null hypothesis, based on the lack of any information about Alice’s intention, is that Alice prepares any pure state with equal probability. Then, the average quantum state measured by Bob turns out to be \( \rho \), and he has to make a new hypothesis about Alice’s intention solely based on the information that the observed density matrix is \( \rho \). The arising ‘lazy’ ensemble is shown to be the alternative hypothesis which minimizes the Type I error.

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Introduction

Consider two parties, Alice and Bob, playing the following game. Alice prepares a pure quantum state according to certain random strategy and then sends it to Bob. Initially Bob possesses no information about Alice’s strategy and thus assumes that Alice performs a completely random choice of pure state, we refer to this statement as a null hypothesis. In this case the average density matrix received by Bob would be be proportional to identity.

Measuring the received states, Bob realizes that the average quantum state emitted by Alice is $\rho$. However, there are infinitely many ensembles which average to $\rho$, and Bob still can not recover the strategy of Alice. Although Bob now possesses some information about Alice’s intentions: if the received density matrix $\rho$ differs from identity, Bob has to make an alternative hypothesis. To specify such a hypothesis, some extra principles must be taken into account. These principles should capture the type of Alice’s behavior.

We might assume that the strategy of Alice is to prepare eigenstates of $\rho$ with given probabilities, but this is just an assumption that Alice is ‘generous’ in providing the accessible information. Or, conversely, Alice might be stingy with the information and thus chooses pure states according to Scrooge distribution [1].

In our game, Bob is reluctant to change his opinion and chooses among Alice’s strategies (which average to $\rho$) the closest to his null hypothesis. By ‘closest’ we mean minimizing the Kullback-Leibler [2] distance between the distributions. This distance is the average likelihood ratio and is associated with the probability of the Type I error$^1$.

Another way for Bob’s reasonings is to assume Alice to be lazy in efforts to prepare the ensemble. These efforts are quantified in terms of differential entropy. Remarkably, as we show in Section 1, both approaches yield the same ensemble [3].

1 Differential entropy and likelihood ratio

First we have to specify a yet vague notion of ‘preparation efforts’ for an ensemble. Following [3] we formulate it in thermodynamic terms, namely,

$^1$To make Type I error means to accept the alternative hypothesis when the null hypothesis is still valid. An example of Type I error would be to conclude that the defendant is guilty, when in fact he or she is innocent.
we quantify these efforts by the difference between the entropy of uniform distribution (that is, our null hypothesis) and the entropy of the ensemble in question. The only obstacle may occur is to define this entropy, let us dwell on it in more detail.

The entropy of a finite distribution \( \{p_i\} \) is given by Shannon formula

\[
S(\{p_i\}) = - \sum p_i \ln p_i
\]

This expression diverges for any continuous distribution: we approximate a continuous distribution \( \mu(x) \) by a discrete one \( \{p_i\} \), calculate its Shannon entropy, but it tends to infinity as we refine the partition. However, we are always interested in the difference between the entropy of the uniform distribution and the distribution \( \mu(x) \) rather than the entropy itself. At each approximation step we calculate this difference, and the appropriate limit always exists. To show it (see, e.g. [5] for details), make a partition of the probability space by \( N \) sets \( \Delta_i \) having equal uniform measure. Then the difference \( E_N \) between the entropies read:

\[
E_N = \ln N - \left( - \sum p_i \ln p_i \right)
\]

where \( p_i = \int_{\Delta_i} p(x) \, dx \). The limit expression \( \lim_{N \to \infty} E_N \) is the differential entropy

\[
S(\mu) = \int \mu(x) \ln \mu(x) \, dx
\]

Remarkably, 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.

\[2\]We are speaking here of mixing entropy [4] of the ensemble rather than about von Neumann entropy of its density matrix.
2 ‘Lazy’ ensembles

The main problem reduces to the following. For given density matrix $\rho$ find a continuous ensemble $\mu$ having minimal differential entropy (1):

$$S(\mu) \rightarrow \min, \quad \int P_{\psi} \mu(\psi) \, d\psi = \rho \tag{2}$$

where $d\psi$ is the unitary invariant measure on pure states normalized to integrate to unity. When there is no constraints in (2), the answer is straightforward—the minimum (equal to zero) is attained on uniform distribution. To solve the problem with constraints, we use the Lagrange multiples method. The appropriate Lagrange function reads:

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

where the Lagrange multiple $\Lambda$ is a matrix since the constraints in (2) are of matrix character. Substituting the expression (1) for $S(\mu)$ and making the derivative of $\mathcal{L}$ over $\mu$ zero, we get

$$\mu(\psi) = e^{-\text{Tr} \, B P_{\psi}} Z(B) \tag{3}$$

where $B$ is the optimal value of the Lagrange multiple $\Lambda$ which we derive from the constraint (2) and the normalizing multiple

$$Z(B) = \int e^{-\text{Tr} \, B P_{\psi}} \, d\psi \tag{4}$$

is the partition function for (3). Substituting the resulting density (3) to the expression (1) for differential entropy we get

$$S = \text{Tr} \, B \rho - \ln Z \tag{5}$$

3 Explicit expressions

First evaluate the partition function (4) in the eigenbasis of $B$. This integral is a special case of the calculations carried out in [6], according to which
\[ Z(B) \text{ reads:} \]

\[ Z(B) = - (n-1)! \sum_{k=1}^{n} \frac{e^{-b_k}}{\prod_{j \neq k} (b_k - b_j)} \]  \hspace{1cm} (6)

where \( b_k \) are the eigenvalues of \( B \). If two or more of them are equal, the appropriate expression is obtained as a limit starting with unequal eigenvalues.

To write down the expression for the eigenvalues \( \lambda_s \) of the density matrix \( \rho \) via \( B \) we could evaluate the integrals

\[ \lambda_s = \langle e_s | \int P_\psi \mu(\psi) \ d\psi | e_s \rangle \]

in the eigenbasis of \( \rho \). Although, like in thermodynamics, we have

\[ \rho = \frac{\partial \ln Z}{\partial B} \]  \hspace{1cm} (7)

which gives the explicit expression for the eigenvalues of the density matrix \( \rho \):

\[ \lambda_s = - \frac{e^{-b_s}}{\prod_{j=1 \atop j \neq s}^{n} (b_s - b_j)} + \sum_{k=1}^{n} \frac{1}{b_s - b_k} \cdot \left( \frac{e^{-b_s}}{\prod_{j=1 \atop j \neq s}^{n} (b_s - b_j)} + \frac{e^{-b_k}}{\prod_{j=1 \atop j \neq k}^{n} (b_k - b_j)} \right) \]

\[ \sum_{k=1}^{n} \frac{e^{-b_k}}{\prod_{j=1 \atop j \neq k}^{n} (b_k - b_j)} \]  \hspace{1cm} (8)

from which we see that the resulting density matrix \( \rho \) remains unchanged when we add a constant to all \( b_k \)-s. That means that the matrix ‘temperature’ parameter \( B \) for the lazy ensemble is defined up to an additive constant (in contrast with classical thermodynamics).

Like in \[ \textbf{1} \], the expression \[ \textbf{9} \] for the partition function can be given the following integral form

\[ Z(B) = - \frac{(n-1)!}{2\pi i} \oint \frac{e^{-z} \ dz}{\det(B - z \mathbf{I})} \]  \hspace{1cm} (9)

where the contour encloses all eigenvalues of \( B \).
So, given a lazy ensemble with the parameter $B$, we have written down the expression for its average density matrix. This expression is well-defined for any matrix $B$. The existence problem remains: given a density matrix $\rho$, is there a lazy ensemble with appropriate parameter $B$ which averages to $\rho$? Similar question—the existence of temperature function—arises in thermodynamics. The idea to solve it is the following: we consider the $n$-dimensional CDF (cumulative density function) of the measure $\mu$ and study the asymptotics of its Laplace transform. As a result, it can be shown that $B$ exists for any full-range density matrix $\rho$.

4 Special case: spin-1/2 particle

In this case the state space has dimension 2. Write down the parameter $B$ in the eigenbasis of the density matrix $\rho$ in a suitable form:

$$B = b \cdot I + \begin{pmatrix} -\beta & 0 \\ 0 & +\beta \end{pmatrix}$$  \hspace{1cm} (10)

Then the expression for partition function reads:

$$Z = e^{-b \cdot e^{\beta} - e^{-x}} = e^{-b} \cdot \frac{\sinh \beta}{\beta}$$  \hspace{1cm} (11)

Calculating the partial derivatives according to (8), we get the following expressions for the coefficients $\lambda_{1,2}$ of the density matrix

$$\lambda_{1,2} = \frac{1}{2} \pm \frac{1}{2} \left( \coth \beta - \frac{1}{\beta} \right) = \frac{1}{2} \pm \delta$$  \hspace{1cm} (12)

where

$$\delta = \frac{1}{2} \left( \coth \beta - \frac{1}{\beta} \right)$$  \hspace{1cm} (13)

Denote by $f(\delta)$ the inverse to $\delta$. Since the $\delta$ is odd and monotone function of $\beta$, its inverse $f$ exists and bears the same properties. Then the matrix $B$ is the following function of the density matrix

$$B = b \cdot I + \begin{pmatrix} f \left( \frac{\lambda_1 - \lambda_2}{2} \right) & 0 \\ 0 & f \left( \frac{\lambda_1 - \lambda_2}{2} \right) \end{pmatrix} = b \cdot I + f \left( \frac{I}{2} - \rho \right)$$
Since the expression (13) for $\rho$ is the independence of the choice of $b$, in two-dimensional case both matrices $B$ and $\rho$ are defined by their mean deviation values $\beta$ and $\delta$, respectively. So, the essential dependence of the matrix ‘temperature’ parameter $B$ from the density matrix $\rho$ is completely captured by the function $f$. Its graph looks as follows.

![Graph showing the function $f$ against $\delta$ and $\beta$.]

5 Lazy ensembles are equilibrium

Like Gibbs ensembles in thermodynamics, the lazy ensembles are equilibrium, namely, the introduced ‘temperature’ parameters $B$ possess the equalizing property. To show it, first introduce the notion of conditional ensemble. In terms of game played by Alice and Bob this means that Bob measures a fixed observable $H$ upon the particles emitted by Alice. Again, he has the uniform distribution as null hypothesis, but the constraint in (2) is of scalar rather than of matrix character. Solving the appropriate variational problem

$$S(\mu) \to \min, \quad \int P_{\psi} \mu(\psi) \, d \psi = \Tr H \rho$$

we obtain

$$\mu_H(\psi) = \frac{e^{-\beta \Tr H \rho}}{Z_H(\beta)}$$

— this ensemble is conditional with respect to given observable $H$.

Consider two quantum systems with state spaces $\mathcal{H}$ and $\mathcal{H}'$, respectively. Let their states initially be $\rho$ and $\rho'$. Then, since we consider a non-interacting
coupling of the systems, the joint density matrix is $\rho \otimes \rho'$ in the tensor product space $\mathcal{H} \otimes \mathcal{H}'$. Let us measure the sum of values of the observables $H$ and $H'$, that is, introduce the observable $\mathbf{H} = H \otimes \mathbf{I} + \mathbf{I} \otimes H'$. The conditional optimal ensemble of separable states with respect to the observable $\mathbf{H}$ is the following distribution

$$\mu_{\mathbf{H}}(\psi \otimes \psi') = \frac{\exp \left[ -\beta_\mathbf{H} \text{Tr} \mathbf{H} \mathbf{P}_{\psi \otimes \psi'} \right]}{Z_\mathbf{H}(\beta_\mathbf{H})}$$

Like in classical thermodynamics, the partition function of the joint system is the product of subsystems’ partition functions:

$$Z_\mathbf{H}(\tau) = \int \int e^{-\tau \text{Tr} \mathbf{H} \mathbf{P}_{\psi \otimes \psi'}} \, d\psi \, d\psi' = \int \int e^{-\tau (\text{Tr} \mathbf{H} \mathbf{P}_{\psi} + \text{Tr} \mathbf{H}' \mathbf{P}_{\psi'})} \, d\psi \, d\psi' = Z_H(\tau) \cdot Z_{H'}(\tau)$$

therefore the equalizing property holds

If $\beta_H \leq \beta_{H'}$ then $\beta_H \leq \beta_\mathbf{H} \leq \beta_{H'}$ \hspace{1cm} (15)

which means that the conditional lazy ensembles are equilibrium and that $\beta$ plays the rôle of temperature parameter.

**Concluding remarks**

Continuous ensembles of pure states proved their relevance in various aspects of quantum mechanics. From the theoretical perspective, they provide the limit cases on which numerical characteristics of density matrices are attained, for instance, the minimal value of accessible information about the state is attained on ‘Scrooge’ ensemble which is a continuous distribution \[\Pi\]. Furthermore, we claim that they are relevant from the operationalistic point of view. Even if we are speaking of preparing discrete ensembles, we must also have in mind that their are unavoidably smeared by various noises and, strictly speaking, we have to deal with continuous distributions.

We use the techniques of continuous ensembles to carry out statistical inference in quantum realm according to the standard scheme: we have an a \textit{priori} hypothesis (we necessarily need it, otherwise there is no way to make
any inference \((7)\), then we obtain some information about the system and have to shift to a new hypothesis.

In our case the null hypothesis is the assumption that any pure state is emitted with equal probability. Then the information is obtained that the average density matrix of the state is \(\rho\). We show how, starting from the ‘minimal effort’ assumption, to guess the strategy of the preparation of the pure states. As a result, we obtain so-called ‘lazy’ ensembles.

These ensembles are also proved to provide the minimal deviation from the null hypothesis. They are described by exponential distributions \((3)\) of pure states averaging to a given density matrix \(\rho\):

\[
\rho = \int \frac{e^{-\langle \psi|B|\psi \rangle}}{Z(B)} \, d\psi
\]

where the matrix parameter \(B\) plays a rôle in some respect similar to temperature, in particular, it is shown to possess the equalizing property. Although we may not treat it as a fully-fledged temperature, for instance, in contrast with classical thermodynamics, it is ambiguously defined up to an arbitrary additive constant. According to formula \((5)\), we can so choose the additive gauge for \(B\) that \(\ln Z\) will vanish and the mean value \(\text{Tr} \, B \rho\) will be equal to the differential entropy of the ensemble, so we may call this matrix parameter \(B\) ‘differential entropy observable’.

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