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Probability measure generated by the superfidelity

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Abstract

We study the probability measure on the set of density matrices induced by the metric defined by using superfidelity. We give the formula for the probability density of eigenvalues. We also study some statistical properties of the set of density matrices equipped with the introduced measure and provide a method for generating density matrices according to the introduced measure.

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1. Introduction

Recent applications of quantum mechanics are based on processing and transferring information encoded in quantum states. Random quantum states can be used to study various effects unique to quantum information theory [1]. This is especially true if one needs to obtain some information about the typical properties of the system in question [2]. In many cases, it is important to quantify to what degree states are similar to the average state or how, on average, a given quantity evolves during the execution of a quantum procedure. The crucial question emerging in this situation is how one should choose a random sample from the set of quantum states.

The aforementioned question can be answered easily in the case of pure quantum states. In this situation there exists a single, natural measure for constructing ensembles of states, namely the Fubini–Study measure. The situation is more complex in the case of mixed quantum states. The probability measure can be introduced using various distance measures between quantum states [2]. By choosing the metric we also choose the probability measure on the set of density matrices. Among the most commonly used metrics we can point out the trace distance, Hilbert–Schmidt distance and Bures distance.

In the analysis of mixed quantum states, Bures distance is the most commonly used metric among the ones mentioned above. It has many important properties [2]. In particular, it is a Riemannian and monotone metric. On the set of pure states it reduces to the Fubini–Study metric [3] and induces the statistical distance in the subset of diagonal density matrices [4].

The main aim of this paper is the analysis of the probability measure on the set of density matrices induced by the metric defined in terms of *superfidelity* [5]. We calculate the formula for the probability density of eigenvalues and study some properties of the set of quantum states equipped with the introduced measure. We also provide a method for sampling random density matrices according to the introduced distribution.

This paper is organized as follows. In section 2, we introduce notation and basic facts used in the following sections. In section 3, we calculate the volume element for the measure generated by the metric based on superfidelity and compare it with the analogous metric based on quantum fidelity. In section 4, we provide a formula for a probability density function on a simplex of eigenvalues. We also calculate the normalization constant in the low-dimensional case. In section 5, we provide a method for sampling density matrices according to the introduced measure. Finally, in section 6 we provide a summary of the presented results.

2. Preliminaries

Let use denote by $\mathcal{M}_N$ the set of density matrices of size N, i.e. $N \times N$ positive-semidefinite matrices with unit trace. The set $\mathcal{M}_N$ forms a convex set in the real space of Hermitian matrices of size N. By Δ we denote the simplex of eigenvalues, i.e. $\Delta = \{\lambda \in \mathbb{R}^N : \lambda_i \geqslant 0, \sum_{i=1}^N \lambda_i = 1\}$.

For two density matrices $\rho, \sigma \in \mathcal{M}_N$, Bures distance can be defined in terms of quantum fidelity [3] as

$$d_{\mathrm{B}}(\rho, \sigma) = \sqrt{2 - 2\sqrt{F(\rho, \sigma)}}, \tag{1}$$

where fidelity, $F(\rho, \sigma) = [\mathrm{tr}\sqrt{\sqrt{\rho}\sigma\sqrt{\rho}}]^2$,provides a measure of similarity on the set of density matrices.

The probability measure on the simplex of eigenvalues generated by the Bures metric was calculated in [6–8]. Various statistical properties of ensembles of quantum states with respect to this measure were discussed in [9].

Bures distance is commonly used in quantum information theory as a natural metric on the set of density matrices. Unfortunately, fidelity used to express d_{B} has some serious drawbacks. In particular, in order to calculate fidelity between two quantum states one needs to compute the square root of the matrix, which is generally a computationally hard task. Also, fidelity cannot be measured directly in the laboratory and thus cannot be used to analyse experiments directly.

These drawbacks motivated the introduction of a new measure of similarity, namely superfidelity [5], defined for $\rho, \sigma \in \mathcal{M}_N$ as

$$G(\rho, \sigma) = \mathrm{tr}\,\rho\sigma + \sqrt{1 - \mathrm{tr}\,\rho^2}\sqrt{1 - \mathrm{tr}\,\sigma^2}. \tag{2}$$

Superfidelity shares many features with fidelity, i.e. it is bounded, symmetric and unitarily invariant. Moreover, it is jointly concave and supermultiplicative. It was proved that superfidelity gives an upper bound for fidelity, $F(\rho, \sigma) \leqslant G(\rho, \sigma)$, where the equality is for $\rho, \sigma \in \mathcal{M}_2$ or in the case where one of the states is pure. It was also shown that, although G is not monotone [10], it can be used to define metric on $\mathcal{M}_N$. Using the correspondence between quantum operations and quantum states, superfidelity can be used to introduce a metric on the set of quantum channels [11]. Superfidelity was also proved to be useful in providing bounds on the trace distance [12] (i.e. distinguishability of states [13]) and as a tool for studying new metrics on the set of quantum states [14].

In the following, we use a metric on the set of density matrices defined for $\rho, \sigma \in \mathcal{M}_N$ as

$$d_G(\rho, \sigma) = \sqrt{2 - 2G(\rho, \sigma)}. \tag{3}$$

Before we discuss further properties of this metric we should stress that the direct analogue of the Bures distance, $d_{\sqrt{G}}(\rho, \sigma) = \sqrt{2 - 2\sqrt{G(\rho, \sigma)}}$, is not a metric. It was shown in [10], that the function $d_{\sqrt{G}}$ generally does not obey the triangle inequality. One should also note that since G is not monotone it cannot be analysed using the Morozova–Čencov–Petz theorem [2].

3. Volume element for the measure

To obtain the probability measure induced by the metric equation (3) one needs to derive the volume element.

The calculations below follow the approach used by Hübner [6]. We begin with the calculation of the line element

$$d_G^2(\rho, \rho + \mathrm{d}\rho) = 2 - 2G(\rho, \rho + \mathrm{d}\rho). \tag{4}$$

We introduce function $A(t) = G(\rho, \rho + t\,\mathrm{d}\rho)$, which allows us to write the line element

$$\sum_{ij} g_{ij}\,\mathrm{d}\rho^i\,\mathrm{d}\rho^j = \frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}t^2}\left[d_G^2(\rho, \rho + t\,\mathrm{d}\rho)\right]\Big|_{t=0} \tag{5}$$

as

$$\sum_{ij} g_{ij}\,\mathrm{d}\rho^i\,\mathrm{d}\rho^j = -A''(t)|_{t=0}. \tag{6}$$

Equivalently, with the use of matrix entries, the line element reads

$$\sum_{ij} g_{ij}\,\mathrm{d}\rho^i\,\mathrm{d}\rho^j = \frac{\left(\sum_i \lambda_i \langle i|\,\mathrm{d}\rho|i\rangle\right)^2}{1 - \sum_i \lambda_i^2} + \sum_i \langle i|(\mathrm{d}\rho)^2|i\rangle. \tag{7}$$

Infinitesimal shift $\rho + \mathrm{d}\rho$ can be decomposed as a shift in eigenvalues and infinitesimal unitary rotation [7]

$$\rho + \mathrm{d}\rho = \rho + \mathrm{d}\Lambda + [\mathrm{d}U, \rho], \tag{8}$$

where $\mathrm{d}\Lambda = \sum_i \mathrm{d}\lambda_i |i\rangle\langle i|$ and $(\mathrm{d}U)^\dagger = -\mathrm{d}U$. Rewriting $\mathrm{d}U$ in computational basis gives

$$\mathrm{d}U = \sum_{j,k} (\mathrm{d}x_{jk} + \mathrm{i}\mathrm{d}y_{jk})|j\rangle\langle k| \tag{9}$$

with real coefficients $\mathrm{d}x_{jk} = -\mathrm{d}x_{kj}$ and $\mathrm{d}y_{jk} = \mathrm{d}y_{kj}$. After some calculations, one obtains

$$\mathrm{tr}\,\mathrm{d}\rho^2 = \sum_i (\mathrm{d}\lambda_i)^2 + 2\sum_{i<j} (\lambda_i - \lambda_j)^2[(\mathrm{d}x_{ij})^2 + (\mathrm{d}y_{ij})^2] \tag{10}$$

and

$$\mathrm{tr}\,\rho\,\mathrm{d}\rho = \sum_i \lambda_i\,\mathrm{d}\lambda_i. \tag{11}$$

Expanding this we obtain the entries of the metric tensor

$$\sum_{ij} g_{ij}\,\mathrm{d}\rho^i\,\mathrm{d}\rho^j = \sum_{i,j}\left(\frac{\lambda_i\lambda_j}{1 - \mathrm{tr}\,\rho^2} + \delta_{ij}\right)\mathrm{d}\lambda_i\,\mathrm{d}\lambda_j \tag{12}$$

$$+\ 2\sum_{i<j} (\lambda_i - \lambda_j)^2[(\mathrm{d}x_{ij})^2 + (\mathrm{d}y_{ij})^2]. \tag{13}$$

To obtain the volume element of the sought measure, one must calculate the appropriate determinant

$$\mathrm{d}V_G = \sqrt{\det\left(\frac{\lambda_i\lambda_j}{1 - \mathrm{tr}\,\rho^2} + \delta_{ij}\right)}\,\mathrm{d}\lambda_1 \ldots \mathrm{d}\lambda_n \tag{14}$$

$$\times \prod_{i<j} 2(\lambda_i - \lambda_j)^2\,\mathrm{d}x_{ij}\,\mathrm{d}y_{ij}. \tag{15}$$

Using the equality

$$\det\left(\frac{\lambda_i\lambda_j}{1-\operatorname{tr}\rho^2}+\delta_{ij}\right)=1+\frac{\operatorname{tr}\rho^2}{1-\operatorname{tr}\rho^2}=\frac{1}{1-\operatorname{tr}\rho^2}, \tag{16}$$

we obtain the expression for the volume element

$$\mathrm{d}V_G=\frac{\mathrm{d}\lambda_1\ldots\mathrm{d}\lambda_n}{\sqrt{1-\sum_i\lambda_i^2}}\prod_{i<j}2(\lambda_i-\lambda_j)^2\,\mathrm{d}x_{ij}\,\mathrm{d}y_{ij}. \tag{17}$$

One can compare the above formulas for the line element with the analogous result for the metric given in terms of fidelity as

$$d_{B'}^2(\rho,\rho+\mathrm{d}\rho)=2\,(1-F(\rho,\rho+\mathrm{d}\rho)). \tag{18}$$

In this case, it is easy to check that the line element is given by the formula

$$d_{B'}^2(\rho,\rho+\mathrm{d}\rho)=\sum_{ij}\frac{|\langle i|\mathrm{d}\rho|j\rangle|^2}{\lambda_i+\lambda_j}. \tag{19}$$

In the one-qubit case, the above formula reads

$$d_{B'}^2(\rho,\rho+\mathrm{d}\rho)=\left(\frac{1}{2\lambda(1-\lambda)}\right)|\mathrm{d}\rho_{11}|^2+|\mathrm{d}\rho_{12}|^2+|\mathrm{d}\rho_{21}|^2, \tag{20}$$

where λ and $1-\lambda$ are eigenvalues of ρ and $\mathrm{d}\rho_{ij}=\langle i|\mathrm{d}\rho|j\rangle$ and we have used the equality $\langle 1|\mathrm{d}\rho|1\rangle=-\langle 2|\mathrm{d}\rho|2\rangle$. This is identical to (7) for $N=2$, which is what one expects since in this case $F(\rho,\sigma)=G(\rho,\sigma)$.

4. Probability density function

In order to obtain the probability measure, we need to specify the normalizing constant. This constant is an inverse of the integral of the volume element $\mathrm{d}V_G$ over the group of unitary matrices and over the simplex of eigenvalues.

4.1. Normalization constant

Integration with respect to $U(N)$ is independent from the integration over the simplex of eigenvalues. We can rewrite equation (17) as

$$\mathrm{d}V_G=\left(\frac{2^{N(N-1)/2}}{\sqrt{1-\sum_i\lambda_i^2}}\prod_{i<j}(\lambda_i-\lambda_j)^2\right)\mathrm{d}\lambda_1\ldots\mathrm{d}\lambda_n\prod_{i\neq j}\mathrm{d}x_{ij}\,\mathrm{d}y_{ij}. \tag{21}$$

After integrating this formula over $U(N)$ we obtain

$$V_G=\Upsilon_N\int_\Delta\left(\frac{2^{N(N-1)/2}}{\sqrt{1-\sum_i\lambda_i^2}}\prod_{i<j}(\lambda_i-\lambda_j)^2\right)\mathrm{d}\lambda_1\ldots\mathrm{d}\lambda_n, \tag{22}$$

where Υ_N is the volume of projective $U(N)$ [4, equation (148)]

$$\Upsilon_N=\frac{\pi^{N(N-1)/2}}{\prod_{d=1}^{N-1}d!} \tag{23}$$

and Δ is the simplex of eigenvalues.

The probability density function on a simplex of eigenvalues is given by

$$f_{\mathrm{G},N}(\lambda)=C_N^{\mathrm{G}}\prod_{i<j}(\lambda_i-\lambda_j)^2\frac{1}{\sqrt{1-\sum_i\lambda_i^2}}, \tag{24}$$

where C_N is a normalization constant. For $N=3$, function $f_{\mathrm{G},N}$ is presented in figure 1(*a*).

Figure 1. Distribution of the eigenvalues for one-qutrit ($N = 3$) density matrices for different probability measures. (*a*) Measure generated by the $\sqrt{1-G}$ metric. (*b*) Measure generated by the Bures metric.

The normalization constant C_N^{G} is the following integral:

$$\frac{1}{C_N^{\mathrm{G}}} = \int_\Delta \prod_{i<j} (\lambda_i - \lambda_j)^2 \frac{1}{\sqrt{1 - \sum_i \lambda_i^2}} \,\mathrm{d}\lambda \tag{25}$$

over the simplex of eigenvalues.

The above integral can be written in terms of the expectation value with respect to the Hilbert–Schmidt measure

$$\frac{1}{C_N^{\mathrm{G}}} = \frac{1}{C_N^{\mathrm{HS}}} E\left[\frac{1}{\sqrt{1 - \operatorname{tr}\rho^2}}\right], \tag{26}$$

where ρ is a random state distributed with the Hilbert–Schmidt measure and

$$C_N^{\mathrm{HS}} = \frac{\Gamma(N^2)}{\prod_{k=1}^N \Gamma(k)\Gamma(k+1)}. \tag{27}$$

The distribution of purity ($\operatorname{tr}\rho^2$) for random states is a subject of much study [15–17].

The probability distribution function of purity is known for Hilbert–Schmidt random states in the case of $N = 2$ and $N = 3$ [16]. Using these results, we can write explicitly normalizing constants

$$C_2^{\mathrm{G}} = \frac{2\sqrt{2}}{3\pi} C_2^{\mathrm{HS}}, \tag{28}$$

$$C_3^{\mathrm{G}} = \frac{432\sqrt{2}}{317\pi} C_3^{\mathrm{HS}}. \tag{29}$$

In the case of $N > 3$, one can use the series expansion of $\frac{1}{\sqrt{1-r}}$ and rewrite the above as

$$\frac{1}{C_N^{\mathrm{G}}} = \frac{1}{C_N^{\mathrm{HS}}} \sum_{k=0}^{\infty} \frac{(2k-1)!!}{k!2^k} E[\operatorname{tr}(\rho^2)^k]. \tag{30}$$

The moments of purity for the Hilbert–Schmidt random state are given by [15, 16]

$$E[(\operatorname{tr}\rho^2)^k] = \frac{N!(N^2-1)!}{(N^2+2N-1)!} \sum_{k_1+\cdots+k_N=k} \frac{k!}{\prod_{i=1}^N k_i!} \tag{31}$$

$$\times \prod_{i=1}^{n} \frac{(n+2k_i-i)!}{(q-i)!i!} \prod_{1\leqslant i<j\leqslant n} (2k_i - i - 2k_j + j). \tag{32}$$

The constant C_N^{G} can be bounded from the above by using the Jensen inequality

$$\frac{1}{C_N^{\mathrm{G}}} = \frac{1}{C_N^{\mathrm{HS}}} E\left[\frac{1}{\sqrt{1-\operatorname{tr}\rho^2}}\right] \tag{33}$$

$$\geqslant \frac{1}{C_N^{\mathrm{HS}}} \frac{1}{\sqrt{1-E[\operatorname{tr}\rho^2]}} = \frac{1}{C_N^{\mathrm{HS}}} \frac{1}{\sqrt{1-\frac{2N}{N^2+1}}}, \tag{34}$$

thus

$$C_N^{\mathrm{G}} \leqslant C_N^{\mathrm{HS}} \sqrt{1-\frac{2N}{N^2+1}}. \tag{35}$$

Since the distribution of purity has the variance given by

$$\sigma^2(\operatorname{tr}\rho^2) = \frac{2(N^2-1)^2}{(N^2+1)^2(N^2+2)(N^2+3)}, \tag{36}$$

it tends to be more concentrated around the mean given by

$$E[\operatorname{tr}\rho^2] = \frac{2N}{N^2+1}, \tag{37}$$

which tends to zero for large N. For small x, function $1/\sqrt{1-x}$ can be approximated with a small error by a linear function. Thus, the Jensen inequality gives a good approximation of C_N^{G} for large values of N, where $\operatorname{tr}\rho^2$ tends to be small.

4.2 Mean purity

Let ρ_G be a random state distributed with measure G. Then, the mean purity is given as

$$E\left[\operatorname{tr}\rho_G^2\right] = \frac{C_N^{\mathrm{G}}}{C_N^{\mathrm{HS}}} E\left[\frac{\operatorname{tr}\rho^2}{\sqrt{1-\operatorname{tr}\rho^2}}\right], \tag{38}$$

where ρ has the Hilbert–Schmidt distribution. Next, we have

$$E\left[\frac{\operatorname{tr}\rho^2}{\sqrt{1-\operatorname{tr}\rho^2}}\right] \geqslant E[\operatorname{tr}\rho^2] E\left[\frac{1}{\sqrt{1-\operatorname{tr}\rho^2}}\right], \tag{39}$$

which follows from the fact that random variables $\operatorname{tr}\rho^2$ and $\frac{1}{\sqrt{1-\operatorname{tr}\rho^2}}$ are associated (see e.g. [18]). Finally, by using equation (26), we obtain

$$E\left[\operatorname{tr}\rho_G^2\right] \geqslant \frac{C_N^{\mathrm{G}}}{C_N^{\mathrm{HS}}} E[\operatorname{tr}\rho^2] E\left[\frac{1}{\sqrt{1-\operatorname{tr}\rho^2}}\right] = E[\operatorname{tr}\rho^2]. \tag{40}$$

From the above equation, we can see that the mean purity for the random state distributed with the measure induced by the superfidelity is greater than the mean purity for the random state distributed with the Hilbert–Schmidt distribution.

5. Generating random states

5.1. One-qubit case

In the case of 2×2 matrices, the density function on the simplex of eigenvalues reads

$$f_{\mathrm{G},2}(\lambda, 1-\lambda) = \frac{2\sqrt{2}}{\pi} \frac{1}{\sqrt{\lambda(1-\lambda)}}. \tag{41}$$

Then, the cumulative probability function for eigenvalues by integrating $f_{G,2}$ over interval $[0, t]$ reads

$$F_{\mathrm{G},2}(t) = \frac{2}{\pi}\left(\sqrt{(1-t)t} - 2\sqrt{(1-t)t^3} + \arcsin\sqrt{t}\right). \tag{42}$$

From the above, we obtain a simple method for generating matrices with the above distribution. First, one must generate eigenvalues of the matrix by inverting the cumulative distribution function and then rotate it by a random unitary matrix distributed with respect to the Haar measure.

5.2. General case

To generate random state of dimension $N > 2$ distributed with the measure induced by the superfidelity, one can use the rejection method (see e.g. [19]).

The probability density function $f_{\mathrm{G},N}$ on a simplex of eigenvalues can be bounded as

$$f_{\mathrm{G},N}(\lambda) \leqslant c f_{\mathrm{B},N}(\lambda), \qquad \forall \lambda \in \Delta, \tag{43}$$

where $f_{\mathrm{B},N}$ is a probability density function generated by the Bures measure [2] (see figure 1(*b*))

$$f_{\mathrm{B},N}(\lambda) = C_N^{\mathrm{B}} \frac{1}{\sqrt{\lambda_1 \ldots \lambda_N}} \prod_{i<j} \frac{(\lambda_i - \lambda_j)^2}{\lambda_i + \lambda_j}. \tag{44}$$

Indeed, we have

$$\sup_{\lambda} \frac{f_{\mathrm{G},N}(\lambda)}{f_{\mathrm{B},N}(\lambda)} = \frac{C_N^{\mathrm{G}}}{C_N^{\mathrm{B}}} \frac{N^{-N/2}(2/N)^{N(N-1)/2}}{\sqrt{1-1/N}} \tag{45}$$

and using the bound for C_N^{G} one can take

$$c = \frac{\sqrt{\frac{N^2-N}{N^2+1}}\,\Gamma(N^2)\pi^{N/2}}{\prod_{i=1}^{N}\Gamma(i) 2^{N(N-1)/2}\Gamma(N^2/2) N^{N^2/2}} \tag{46}$$

as the constant in equation (43).

In order to generate a matrix distributed according to the measure induced by the superfidelity, one needs to generate a random matrix X distributed with the Bures measure [20] and a random number u distributed uniformly over the unit interval [0, 1]. To accept X as a matrix distributed according to the measure induced by the superfidelity, we check if $u \leqslant \frac{1}{c}\frac{f_{\mathrm{G},N}(X)}{f_{\mathrm{B},N}(X)}$ holds. Unfortunately, constant c increases very rapidly with N and thus this method does not work very efficiently for large N.

6. Summary

We have analysed random density matrices distributed according to the probability measure induced by superfidelity. We have derived the formula for the probability density of eigenvalues according to this measure. We have also shown that random states distributed according to this measure have mean purity larger than in the case of the Hilbert–Schmidt measure. We also provide a method for generating random matrices according to the introduced distribution.

We conclude by saying that there is no single, naturally distinguished probability measure in the set of density matrices. The question is how one should choose a random density matrix if one needs to obtain some information about the typical properties of the system. In this paper, we have presented a new probability measure defined on the basis of superfidelity, which can be used in studying the properties of the set of density matrices. The metric based on superfidelity has properties which makes it useful for quantifying the distance between quantum states. Superfidelity shares many properties with quantum fidelity, (e.g. bounds, symmetry, unitary invariance, concavity), but it is much easier to calculate than fidelity, and furthermore, there exists a scheme to measure it between arbitrary mixed states [5].

Still there are some problems which require further investigation. The first is the calculation of the exact formula for the normalization constant for the probability density function. This is directly related to the distribution of purity for measures induced by the partial trace [16, 15]. The second problem is the inefficient method of sampling random states with the introduced measure, which could be used for numerical studies of the geometry of quantum states [2, 21, 22].

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