On a Geometric Structure of Pure Multi-qubit Quantum States and Its Applicability to a Numerical Computation

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Abstract

For one-qubit pure quantum states, it is already proved that the Voronoi diagrams with respect to two distances — Euclidean distance and the quantum divergence — coincide. This fact is a support for a known method to calculate the Holevo capacity. To consider an applicability of this method to quantum states of a higher level system, it is essential to check if the coincidence of the Voronoi diagrams also occurs. In this paper, we show a negative result for that expectation. In other words, we mathematically prove that those diagrams no longer coincide in a higher dimension. That indicates that the method used in one-qubit case to calculate the Holevo capacity might not be effective in a higher dimension.

1. Introduction

The movement of trying to apply quantum mechanics to information processing has given vast research fields in computer science. Especially among them quantum information theory is developed as one of the richest research fields. Some aspect of quantum information theory is to investigate a kind of distance between two different quantum states. Depending on the situation, several distances are defined in quantum states.

The significance of quantum information theory is also due to its rich variety of mathematical methods used there. Especially, geometric interpretation of quantum states has been an important theme. The researches from that kind of view are categorized as “quantum information geometry.” Actually some properties of a space of quantum states as a metric space have been researched in some contexts.

A quantum channel is a channel that transfers quantum information. Mathematically it is represented as an affine transformation between two Hilbert spaces, each of which is a representation of quantum states. One of the main problems in the quantum information theory is how well a quantum channel transfers information. Especially, one of the most important indications that show a capacity of quantum channel is the Holevo capacity. Intuitively speaking, the Holevo capacity indicates how much the channel preserves the size of the space of the quantum states. The measure used here is called the quantum divergence, which is a kind of a distance of two quantum states.

Oto et al. showed that the Holevo capacity of one-qubit states can be numerically computed by considering the image of the source points of the channel. In that paper, points in pure states are plotted so that they are almost uniformly distributed with respect to the Euclidean distance. Here pure states are important because they appear in the boundary of the convex object which corresponds to the whole space of the quantum states. Although their images...
are dealt in a context of the divergence, the algorithm is reasonable because the spaces of pure quantum states with respect to the two distances have the same structure. In other words, in pure states, uniformly distributed points in the world of the Euclidean distance is also uniformly distributed with respect to the divergence. The authors showed that fact mathematically considering Voronoi diagrams.

A natural question that arises after this story is “What happens in a higher level systems?” If you could say the same thing in a higher dimension, the method used in the one-qubit case for a calculation of the Holevo capacity might be applied to a general case. However, unfortunately we found it is not the case. The main result of this paper is the fact that in a higher dimension, the two distance spaces do not coincide in a higher dimension. Additionally we give some examples for the understanding of the structure.

The rest of this paper is organized as follows. First in Section 2 we give some basic facts in quantum information theory. In Section 3 we explain briefly the known fact about one-qubit quantum space. Section 4 is the main part of this paper, where we show some workout for a higher level case and give some illustrative examples. Lastly in Section 5 we summarize the result and give it some discussion.

2. Preliminaries

2.1. Parameterization of quantum states

In quantum information theory, a density matrix is representation of some probabilistic distribution of states of particles. A density matrix is expressed as a complex matrix which satisfies three conditions: a) It is Hermitian, b) the trace of it is one, and c) it must be semi-positive definite. We denote by $\mathcal{S}(\mathbb{C}^d)$ the space of all density matrices of size $d \times d$. It is called “d-level system.”

Especially in two-level system, which is often called “one-qubit system”, the conditions above are equivalently expressed as

$$
\rho = \frac{1 + z}{2} \begin{pmatrix}
\frac{1}{2} + izy & x + iy \\
\frac{1}{2} - izy & \frac{1}{2} - x - iy
\end{pmatrix},
$$

$$
x^2 + y^2 + z^2 \leq 1, \quad x, y, z \in \mathbb{R}.
$$

The parameterized matrix correspond to the conditions a) and b), and the inequality correspond to the condition c).

There have been some attempt to extend this Bloch ball expression to a higher level system. A matrix which satisfies only first two condition, Hermitianness and unity of its trace, is expressed as:

$$
\rho = \begin{pmatrix}
\xi_1 + \frac{1}{d} & \xi_2 - i\xi_{d+1} & \cdots & \xi_{3d-4} - i\xi_{3d-3} \\
\xi_2 + i\xi_{d+1} & \frac{2}{d} & \cdots & \xi_{3d-2} - i\xi_{3d-2} \\
\cdots & \cdots & \cdots & \cdots \\
\xi_{3d-4} + i\xi_{3d-3} & \xi_{3d-2} + i\xi_{3d-1} & \cdots & \frac{2}{d} - \sum_{i=1}^{d-1} \xi_i + \frac{1}{d} \\
\xi_{3d-2} - i\xi_{3d-1} & \xi_{3d-3} - i\xi_{3d-2} & \cdots & \frac{2}{d} - \sum_{i=1}^{d-1} \xi_i + \frac{1}{d}
\end{pmatrix},
\xi_i \in \mathbb{R}.
$$

Actually, any matrix which is Hermitian and whose trace is one is expressed this way with some adequate $\{\xi_i\}$. This condition doesn’t contain a consideration for a semi-positivity. To add the condition for a semi-positivity, it is not simple as in one-qubit case, and we have to consider complicated inequalities. Note that this is not the only way to parameterize all the density matrices, but it is reasonably natural way because it is natural extension of one-qubit case and has a special symmetry.

Additionally our interest is a pure state. A pure state is expressed by a density matrix whose rank is one. A density matrix which is not pure is called a mixed state. A pure state is naturally parameterized by a set of $\{\xi_i\}$ and also has a geometrically special meaning because it is natural extension of one-qubit case and has a special symmetry.

We define the log of density matrix. When eigenvalues of $\rho$ are diagonalized with a unitary matrix $X$ as

$$
\rho = X \begin{pmatrix}
\lambda_1 \\
\lambda_2 \\
\vdots \\
\lambda_d
\end{pmatrix} X^*,
$$

the log of $\rho$ is defined as

$$
\log \rho = X \begin{pmatrix}
\log \lambda_1 \\
\log \lambda_2 \\
\vdots \\
\log \lambda_d
\end{pmatrix} X^*.
$$
The quantum divergence is one of measures that show the difference of two quantum states. The quantum divergence of the two states $\sigma$ and $\rho$ is defined as

$$ D(\sigma||\rho) = \text{Tr} \sigma (\log \sigma - \log \rho). \quad (6) $$

Note that though this has some distance-like properties, it is not commutative, i.e. $D(\sigma||\rho) \neq D(\rho||\sigma)$. The divergence $D(\sigma||\rho)$ is not defined when $\rho$ does not has a full rank, while $\sigma$ can be non-full rank. This is because for a non-full rank matrix, a log of zero appears in the definition of the divergence. However, since $0 \log 0$ is naturally defined as $0$, some eigenvalues of $\sigma$ can be zero.

A quantum channel is the linear transform that maps quantum states to quantum states. In other words, a linear transform $\Gamma : M(\mathbb{C}; d) \rightarrow M(\mathbb{C}; d)$ is a quantum channel if $\Gamma(\mathcal{S}(\mathbb{C}^d)) \subset \mathcal{S}(\mathbb{C}^d)$.

The Holevo capacity $\mathcal{C}$ of this quantum channel is known to be equal to the maximum divergence from the center to a given point and the radius of the smallest enclosing ball. The Holevo capacity $\mathcal{C}(\Gamma)$ of a 1-qubit quantum channel $\Gamma$ is defined as

$$ \mathcal{C}(\Gamma) = \inf_{\sigma \in \mathcal{S}(\mathbb{C}^d)} \sup_{\rho \in \mathcal{S}(\mathbb{C}^d)} D(\Gamma(\sigma)||\Gamma(\rho)). \quad (7) $$

### 3. One-qubit case

Our first motivation to investigate a Voronoi diagram in quantum states is the numerical calculation of the Holevo capacity for one-qubit quantum states [7]. In that paper, some points are plotted in the source of channel, and it is assumed that just thinking of the images of plotted points is enough for approximation. Actually, the Holevo capacity is reasonably approximated taking the smallest enclosing ball of the images of the points. More precisely, the procedure for the approximation is the following:

1. Plot equally distributed points on the Bloch ball which is the source of the channel in problem.
2. Map all the plotted points by the channel.
3. Compute the smallest enclosing ball of the image with respect to the divergence. Its radius is the Holevo capacity.

In this procedure, step 3 uses a farthest Voronoi diagram. That is the essential part to make this algorithm effective because Voronoi diagram is the known fastest tool to seek a center of a smallest enclosing ball of points.

However, when you think about the effectiveness of this algorithm, there might arise a question about its reasonableness. Since the Euclidean distance and the divergence are completely different, Euclideanally uniform points are not necessarily uniform with respect to the divergence. So why does this mechanism work correctly? You cannot say the approximation is good enough unless uniformness of the image of points is guaranteed. That concern is overcome by comparing the Voronoi diagrams. The following theorem is more precise description [3].

**Theorem 1.** Suppose that $n$ one-qubit pure states are given, the following Voronoi diagrams of them are equivalent:

1. The Voronoi diagram in pure states obtained by taking a limit of the diagram with respect to the divergence
2. The Voronoi diagram on the sphere with respect to the ordinary geodetic distance
3. The section of the three-dimensional Euclidean Voronoi diagram with the sphere

Note that although the divergence is not defined in the pure states, we can consider the limit of the diagram with respect to the divergence in the pure states. In this paper, Voronoi sites are plotted as a first argument of the divergence $D(\cdot||\cdot)$. From now on, when we say “Voronoi diagram with respect to the divergence”, it means a limit of a diagram with sites in the first argument of $D(\cdot||\cdot)$.

### 4. Higher level case

In this section, we show that the coincidence which happens in one-qubit case never occurs in a higher level case. To show it, it is enough to look at some section of the diagrams with some hyperplain. If the diagrams do not coincide in the section, you can say they are different.

Suppose that $d \geq 3$ and that the space of general quantum states is expressed as Equation [4], and let us think the section of it with a hyperplain:

$$ \xi_{d+2} = \xi_{d+3} = \cdots = \xi_{d^2-1}. \quad (8) $$

Then the section is expressed as:

$$ \rho = \begin{pmatrix}
\frac{\xi_1+1}{2} & \frac{\xi_2-\xi_{d+1}}{d} & \cdots & 0 \\
\frac{\xi_{d+1}+1}{2} & \frac{\xi_{d+2}-\xi_{2d+1}}{d} & \cdots & 0 \\
\vdots & \ddots & \ddots & \vdots \\
0 & \cdots & \frac{\xi_{d^2-1}+1}{d} & \frac{\xi_{d^2}-\xi_{d^2+1}}{d}
\end{pmatrix}. \quad (9) $$

The elements of this matrix are 0 except diagonal, $(0,1)$, and $(1,0)$ elements. This matrix is diagonalized with a unitary
matrix as:

\[
\rho = \begin{pmatrix}
X & 0 \\
0 & I_{d-2}
\end{pmatrix}
\begin{pmatrix}
\lambda_1 & \frac{\xi_1 + \xi_2 + 2}{2d} + \frac{r}{2} \\
\lambda_2 & \frac{\xi_1 + \xi_2 + 2}{2d} - \frac{r}{2}
\end{pmatrix}
\times \begin{pmatrix}
X^* & 0 \\
0 & I_{d-2}
\end{pmatrix},
\]

where

\[
r = \sqrt{\frac{(\xi_1 - \xi_2)^2}{2d^2} + \xi_3^2 + \xi_{d+1}^2},
\]

\[
\lambda_1 = \frac{\xi_1 + \xi_2 + 2}{2d} + \frac{r}{2},
\]

\[
\lambda_2 = \frac{\xi_1 + \xi_2 + 2}{2d} - \frac{r}{2}
\]

\[
X = \begin{pmatrix}
\frac{\xi_1 - \xi_{d+1}}{2} & \frac{\xi_2 - \xi_{d+1}}{2} \\
\frac{\xi_2 - \xi_1}{2d} + \frac{r}{2} & \frac{\xi_2 - \xi_1}{2d} - \frac{r}{2}
\end{pmatrix},
\]

\[
R_+ = \frac{\xi_1^2 + \xi_{d+1}^2}{4} + \left( \frac{\xi_2 - \xi_1}{2d} + \frac{r}{2} \right)^2,
\]

\[
R_- = \frac{\xi_1^2 + \xi_{d+1}^2}{4} + \left( \frac{\xi_2 - \xi_1}{2d} - \frac{r}{2} \right)^2.
\]

Case 1 (only \(d\)-th raw of the matrix is non-zero)

\[
\xi_1 = \xi_2 = \cdots = \xi_{d-1} = -1, \quad \xi_d = \xi_{d+1} = 0.
\]

Case 2 (only one \(i\)-th raw (\(3 \leq i \leq d-1\)) is non-zero)

\[
\xi_1 = \xi_2 = -1, \quad \xi_3 = \xi_{d+1} = 0,
\]

all of \(\xi_j (3 \leq j \leq d-1)\) are \(-1\) except one (let its index to be \(k\)) and \(\xi_k = d-3\).

Case 3 (only \(\lambda_2\) is non-zero)

\[
\xi_1 + \xi_2 = d - 2, \quad \xi_2 - \xi_1 \frac{d^2}{4} + \frac{d^2}{4} (\xi_3^2 + \xi_{d+1}^2) = 1,
\]

\[
\xi_3 = \xi_4 = \cdots = \xi_{d-1} = -1.
\]

Note that it is impossible that only \(\lambda_1\) is non-zero. In both Case 1 and Case 2, the set of points that satisfies the condition is just one point, so our main interest is Case 3. The set of points that satisfies this condition is a manifold. Actually, Case 3 satisfies

\[
\frac{(d - 2 - 2\xi_1)^2}{4} + \frac{d^2}{4} (\xi_3^2 + \xi_{d+1}^2) = 1,
\]

and this is an ellipsoid.

Then we prepare for workout of the divergence. The log of \(\rho\) is expressed as:

\[
\log \rho = \begin{pmatrix}
X & 0 \\
0 & I_{d-2}
\end{pmatrix}
\begin{pmatrix}
\log \lambda_1 & \log \frac{\xi_1 + \xi_2 + 2}{2d} \\
\log \lambda_2 & \log \frac{\xi_1 + \xi_2 + 2}{2d} - \frac{r}{2}
\end{pmatrix}
\times \begin{pmatrix}
X^* & 0 \\
0 & I_{d-2}
\end{pmatrix},
\]

Thus, we obtain

\[
\text{Tr} \sigma \log \rho = \frac{\eta_1 + 1}{d} \left[ \log \lambda_1 + \log \lambda_2 \right] + \eta_2 \left[ \log \lambda_1 + \log \lambda_2 \right] + \eta_{d+1} \left[ \log \lambda_1 + \log \lambda_2 \right] + \frac{1 - \xi_1 - \xi_2}{d}.
\]

With some workout, we get

\[
R_+ = r \left( \frac{\xi_2 - \xi_1}{2d} + \frac{r}{2} \right), \quad R_- = -r \left( \frac{\xi_2 - \xi_1}{2d} - \frac{r}{2} \right).
\]

Using these fact and the assumption \(\eta_1 + \eta_2 = \xi_1 + \xi_2 = d - 2\), we get

\[
\text{Tr} \sigma \log \rho = \left[ \frac{\eta_1 + \eta_{d+1} + \xi_1 + \xi_{d+1}}{2r} \right] \log \lambda_1 + \left[ \frac{\eta_1 + \eta_{d+1} + \xi_1 + \xi_{d+1}}{2r} \right] \log \lambda_2
\]

\[
+ \frac{1 - \xi_1 - \xi_2}{d} \log \lambda_1 \lambda_2.
\]
Next we think of a Voronoi diagram with only two regions for simplicity. It is enough for our objective. Let \( \sigma \) and \( \tilde{\sigma} \) be two sites, and suppose that \( \rho \) moves along the boundary of the Voronoi regions. Suppose that \( \sigma \) and \( \tilde{\sigma} \) are parameterized by \( \{ \eta_j \} \) and \( \{ \tilde{\eta}_j \} \) respectively in the same way as \( r \).

We consider what happens if \( r(0 \leq r < 1) \) is fixed and the following holds:

\[
\xi_1 + \xi_2 = d - 2, \quad \xi_3 = \cdots = \xi_{d-1} = -1. \tag{23}
\]

The condition \( 0 \leq r < 1 \) means that \( \rho \) is semi-positive and not a pure state while \( r = 1 \) in pure states. In other words, we regard that \( \rho \) is on the same ellipsoid obtained by shrinking the ellipsoid expressed by Equation (18). These settings are in order to take a limit of a diagram to get a diagram in the pure states. Taking the limit \( r \to 1 \), we can get a condition for pure states. This procedure is analogous to the method used in \([3]\).

Now to think of the shape of boundary, we have to solve the equation

\[
D(\sigma \parallel \rho) = D(\tilde{\sigma} \parallel \rho), \tag{24}
\]

and this is equivalent to

\[
\text{Tr} (\sigma - \tilde{\sigma}) \log \rho = 0. \tag{25}
\]

Using Equation (22), we obtain

\[
\text{Tr} (\sigma - \tilde{\sigma}) \log \rho = \frac{1}{d^2} \left[ (\eta_d - \tilde{\eta}_d)\xi_d + (\eta_{d+1} - \tilde{\eta}_{d+1})\xi_{d+1} + \frac{4(\eta_1 - \tilde{\eta}_1)(\xi_1 - \frac{d-2}{d^2})}{d^2} \right] \times \log \frac{\lambda_1}{\lambda_2}. \tag{26}
\]

Here when \( r = 0 \), this is zero because \( \lambda_1/\lambda_2 = 1 \). In that case, \( \rho \) can take only one point, but we do not have to care about this case because we are going to take the limit \( r \to 1 \). From now on, we suppose \( r > 0 \) and that means \( \lambda_1/\lambda_2 \neq 1 \).

Hence we get the following equation that holds in the boundary of the Voronoi diagram:

\[
(\eta_d - \tilde{\eta}_d)\xi_d + (\eta_{d+1} - \tilde{\eta}_{d+1})\xi_{d+1} + \frac{4(\eta_1 - \tilde{\eta}_1)(\xi_1 - \frac{d-2}{d^2})}{d^2} = 0. \tag{27}
\]

Consequently, taking the limit \( r \to 1 \), we get Equation (22) as the expression of the boundary in pure states.

A careful inspection of Equation (27) tells us a geometric interpretation of this boundary. We obtain the following theorem:

**Theorem 2.** On the ellipsoid of the pure states which appears in the section with the hyperplain defined above, if transferred by a linear transform which maps the ellipsoid to a sphere, the Voronoi diagram with respect to the divergence coincides with the one with respect to the Euclidean distance.

**Proof.** Think of the affine transform defined by

\[
\begin{pmatrix}
x \\
y \\
z
\end{pmatrix} = \begin{pmatrix}
\xi_1 - \frac{d-2}{d^2} \\
\xi_d \\
\xi_{d+1}
\end{pmatrix}, \tag{28}
\]

then Equation (27) is expressed as

\[
x'(x - x) + y'(y - y) + z'(z - z) = 0, \tag{29}
\]

while Equation (18) becomes

\[
x^2 + y^2 + z^2 = 1. \tag{30}
\]

Thus when \( (x, y, z) \) and \( (x', y', z') \) are fixed, the point \( (x', y', z') \) which stand for \( \eta \) runs along the geodesic. \( \square \)

Now we work out the Voronoi diagram with respect to Euclidean distance. Under the assumption above, the Euclidean distance is expressed as

\[
d(\sigma, \rho) = (\eta_1 - \xi_1)^2 + (\eta_2 - \xi_2)^2 + (\eta_d - \xi_d)^2 + (\eta_{d+1} - \xi_{d+1})^2
\]

\[
= 2(\eta_1 - \xi_1)^2 + (\eta_d - \xi_d)^2 + (\eta_{d+1} - \xi_{d+1})^2, \tag{31}
\]

and we get the equation for boundary as

\[
d(\sigma, \rho) - d(\tilde{\sigma}, \rho) = -4(\eta_1 - \tilde{\eta}_1)\xi_1 - 2(\eta_d - \tilde{\eta}_d)\xi_d - 2(\eta_{d+1} - \tilde{\eta}_{d+1})\xi_{d+1} + 2(\eta_1^2 - \tilde{\eta}_1^2) + (\eta_d^2 - \tilde{\eta}_d^2) + (\eta_{d+1}^2 - \tilde{\eta}_{d+1}^2) = 0. \tag{32}
\]

By comparing the coefficients of \( \xi_1, \xi_d, \xi_{d+1} \), we can tell that the boundaries expressed by Equation (24) and (22) are different. To show how different they are, we give some examples in the rest of this section.

**Example 1.** Suppose that \((\eta_1, \eta_d, \eta_{d+1}) = (d-1, 0, 0)\) and \((\tilde{\eta}_1, \tilde{\eta}_d, \tilde{\eta}_{d+1}) = (-1, 0, 0)\), then the boundary is a) \( \xi_1 = \frac{d-2}{d^2} \) for the divergence, and b) \( \xi_1 = 1 \) for the Euclidean distance. Fig. 1 shows this example for \( d = 5 \). In Fig. 1 Voronoi sites are located on the top and the bottom of the ellipsoid. The two diagrams are the same when \( d = 4 \), but are different otherwise.

**Example 2.** Suppose that \((\eta_1, \eta_d, \eta_{d+1}) = (0, 1, 0)\) and \((\tilde{\eta}_1, \tilde{\eta}_d, \tilde{\eta}_{d+1}) = (0, -1, 0)\), then the boundary is, for both the divergence and Euclidean distance, expressed by \( \xi_{d+1} = 0 \).
Figure 1. An example of a Voronoi diagram with two sites. The figure on the left is the diagram by the divergence, and the figure on the right is the diagram by the Euclidean distance.

**Example 3.** Consider the Voronoi diagram with the following eight sites:

\[
\begin{aligned}
&\left( \frac{d-2}{2}, \frac{d}{2\sqrt{3}}, \pm \frac{1}{\sqrt{3}}, \pm \frac{1}{\sqrt{3}} \right), \\
&\left( \frac{d-2}{2} - \frac{d}{2\sqrt{3}}, \pm \frac{2}{3}, 0 \right), \\
&\left( \frac{d-2}{2} - \frac{d}{2\sqrt{3}}, 0, \pm \frac{2}{3} \right),
\end{aligned}
\]  

(33)

where ±’s mean all the possible combinations. Then the Voronoi diagrams look like Fig. 2. This figure is also for \(d = 5\). Obviously they are different.

Figure 2. An example of a Voronoi diagram with eight sites. The left is the diagram by the divergence, and the right is by the Euclidean distance.

5. Conclusion

We proved that in \(n\)-level system for \(n \geq 3\), the Voronoi diagrams with respect to the divergence and Euclidean distance do not coincide. Additionally we obtained an explicit expression of some section of the boundary of the Voronoi diagram with respect to the divergence. The section is an ellipsoid and after some linear transform, the boundary becomes a geodesic on a sphere. Interestingly this is similar to the whole space of the one-qubit states even though a space of higher level has much more complicated geometric structure.

We also showed some geometric structure concerning how pure states appear in a whole quantum states. Although our result is very restricted, we believe this will be a help for further understanding of the structure. To relax the restriction is our future work.

The result shown in this paper depends on the parameterization of density matrix. The parameterization used in this paper, though it is very natural one, is not unique. To think of another parameterization is another future work.

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