Some Thoughts for Oscar

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Intro

What does it mean for a two qubit quantum state sampling to be random? As you see in the paper I sent (link here) there are a number of ways to conceptualize the "space" that two-qubit quantum states take up, with all of them boiling down to some conception of "distance" between $n \times n$ matrices. One of the most common definitions of distance (heavily used in the paper) is the Hilbert-Schmidt distance between points, defined as

$$HSD(A,B) = ||A - B||_2 \tag{1}$$

Where the Hilbert-Schmidt norm is

$$||A||_2 = \sqrt{\langle A|A\rangle} \tag{2}$$

And the Hilbert-Schmidt inner product of two matrices is defined as

$$\langle A|B\rangle = \text{Tr}(A^{\dagger}B)$$
 (3)

My thoughts going forward are a bit half-baked but I think I am onto something quite interesting, so I'll do my best to explain. Basically the tactic here is

- 1. Define the properties of the density matrix
- 2. Define a basis of matrices
- 3. Restrict the components of the vector space to yield valid (kinda) density matrices \mathbf{x}
- 4. Create a uniform distribution of vectors within that space of valid matrices

My Strategy

First, the properties of the density matrix (mathematically). Any matrix ρ that satisfies

$$\rho = \rho^{\dagger} \tag{4}$$

$$Tr(\rho) = 1 \tag{5}$$

$$\rho \ge 0 \tag{6}$$

is a valid density matrix. Note that eq. (6) is just saying that the matrix is semidefinite positive (no negative eigenvalues).

I was feeling inspired by the Bloch-vector parameterization approach mentioned in the paper, however if you actually try to implement the approach they talked about you'll find almost no Bloch-vectors yield a valid density matrix. I got to thinking about the basis $\{\mathbb{I}, \sigma_x, \sigma_y, \sigma_z\}$ for 2×2 hermitian matrices, and realized we could construct a similar basis for 4×4 hermitian matrices:

$$\begin{split} \{e_i\} &= \{ \mathbb{I} \otimes \mathbb{I}, \mathbb{I} \otimes \sigma_x, \mathbb{I} \otimes \sigma_y, \mathbb{I} \otimes \sigma_z, \\ \sigma_x \otimes \mathbb{I}, \sigma_x \otimes \sigma_x, \sigma_x \otimes \sigma_y, \sigma_x \otimes \sigma_z \\ \sigma_y \otimes \mathbb{I}, \sigma_y \otimes \sigma_x, \sigma_y \otimes \sigma_y, \sigma_y \otimes \sigma_z \\ \sigma_z \otimes \mathbb{I}, \sigma_z \otimes \sigma_x, \sigma_z \otimes \sigma_y, \sigma_z \otimes \sigma_z \} \end{split}$$

Although looking really silly, this basis has some really stupidly wonderful properties for describing the density matrices. Plus, since it is a basis for Hermitian matrices eq. (4) is automatically satisfied by any linear combination of e_i . Really quick, lets define $\mathbf{e} = \begin{pmatrix} e_0 & \cdots & e_{n^2-1} \end{pmatrix}^T$ so that any linear combination of the basis matrices is $\mathbf{v} \cdot \mathbf{e}$ for $\mathbf{v} \in \mathbb{R}^{n^2}$.

Another wonderful property of this basis is that $\operatorname{Tr}(e_i) = 0$ for $i \neq 0$, and $\operatorname{Tr}(e_0) = n^2$ (for *n*-qubit density matrices). This means that if we require $v_0 = n^{-2}$, then $\operatorname{Tr}(\mathbf{v} \cdot \mathbf{e}) = 1$, satisfying eq. (5). From here on out, I'm going to be *very sloppy* about if I'm referring to the full $\mathbf{v} \in \mathbb{R}^{n^2}$ or dropping the first component and referring to $\mathbf{v} \in \mathbb{R}^{n^2-1}$, sorry about that!

Furthermore, we can discuss the bounds of the components v_i very nicely, since all σ_i have eigenvalues of ± 1 , we must have $v_i \in [-1, 1]$.

To show the above fact robustly, we have to make note of perhaps the most important and useful fact of this basis: all e_i are **orthogonal** under the Hilbert-Schmidt inner product! This is why we can restrict v_i so cleanly, since

$$\langle e_j \rangle = \operatorname{Tr}(e_j \rho)$$

$$= \operatorname{Tr}(e_j (\mathbf{e} \cdot \mathbf{v}))$$

$$= \operatorname{Tr} \left(e_j \sum_i e_i v_i \right)$$

$$= \sum_i v_i \operatorname{Tr}(e_j e_i)$$

$$= \sum_i v_i \operatorname{Tr} \left(e_j^{\dagger} e_i \right)$$

$$\langle e_j \rangle = v_j$$

Where the second to last line follows since all e_i are Hermitian so $e_i = e_i^{\dagger}$. Since we know that the expectation value for any σ_i is ± 1 , the expectation value for $\sigma_i \otimes \sigma_j$ (or equivalently, any e_k) is also ± 1 , which restricts the value of v_i thanks to the math shown above.

But here is the real kicker. Consider the Hilbert-Schmidt norm of one of these matrices.

$$||\mathbf{v} \cdot \mathbf{e}||_{2} = \sqrt{\text{Tr}\{(\mathbf{v} \cdot \mathbf{e})^{\dagger}(\mathbf{v} \cdot \mathbf{e})\}}$$

$$= \sqrt{\text{Tr}\left\{\sum_{i} \sum_{j} v_{i} v_{j} e_{i}^{\dagger} e_{j}\right\}}$$

$$= \sqrt{\sum_{i} \sum_{j} v_{i} v_{j} \text{Tr}\left\{e_{i}^{\dagger} e_{j}\right\}}$$

$$= \sqrt{\sum_{i} \sum_{j} v_{i} v_{j} \delta_{ij}}$$

$$= \sqrt{\sum_{i} v_{i}^{2}}$$

$$= ||\mathbf{v}||$$

In fact, the orthonormal vector space described by the coefficients of these spin matrices perfectly encodes the Hilbert-Schmidt distances between matrices as the Euclidian norm of the difference of two vectors.

This fact is super convenient, because now we can just generate an even volumetric distribution of vectors $\mathbf{v} \in \mathbb{R}^{15}$ and we will satisfy a even spacing according to the Hilbert-Schmidt norms, depending on how you want to define an "even spacing."

Conclusion and Outstanding Questions

Putting it all together: Now we know that we can generate these \mathbf{v} that live inside the unit-cube in \mathbb{R}^{15} (15 for the $n^2 = 16$ basis matrices, -1 since $v_0 = n^{-2}$ is predetermined) and each correspond to a unique density matrix¹ and do a fantastic job of encoding Hilbert-Schmidt distances as Euclidian norms in \mathbb{R}^{15} .

Perhaps the most important note at this point is that eq. (6), is not automatically satisfied by this generation approach, however it is *far* more likely to be satisfied (as I learned from my code implementation) than it is to be satisfied with the Bloch-vector parameterization. However, that calls into question: why is it not always satisfied?

Here are my outstanding questions:

1. Why is eq. (6) not always satisfied? What is the subspace in \mathbb{R}^{15} that is traced out by only valid density matrix vectors? What does it look like? What properties does it have?

 $^{^1}$ I didn't show this fact, but it is well-known that a basis for n qubit density matrices must have at least n^2-1 components. Since we have exactly that many components, there are no extra degrees of freedom.

- 2. For a one-qubit analogue to this approach, $||\mathbf{v}|| \leq 1$ is the correct bound for \mathbf{v} . I'm almost certain the same thing holds here, and I can think of one way to prove it (using uncertainty principles) but it would help me sleep at night to know this is definitely the case.
- 3. Just because an even volumetric distribution of $\langle \sigma_i \rangle$ for a single qubit implies a random sampling doesn't necessarily mean that the same holds for $n \geq 2$ qubits. I'm wondering if there is a way to be more rigorous about this?