

The result about barren plateaus here is from the paper [3]; I have only changed the presentation, since there everything is discussed with reference to the parametrised circuit, whereas here everything is treated just in terms of the unitary group. Many thanks to Leonard Wossnig for introducing me to this work.

NISQ and unitary 2-designs. One major current theme in quantum computation is NISQ — noisy intermediate-scale quantum technology. The idea is that we don't have a universal quantum computer yet, and probably won't have one in the near future; so, until then, what can we do with the technology we do have?

One near-term goal is to demonstrate *quantum supremacy* — that is, to show that a quantum device can solve a problem that a classical computer would be incapable of solving. It's not necessary that this problem be useful.

One approach suited to current technology is to consider quantum circuits with parametrised local gates. When parameters are chosen and the quantum circuit evaluated, a unitary transformation is performed. Choosing the parameters at random (according to the uniform distribution, say) therefore induces a distribution on the space $U(d)$ of n -qubit unitary operators (where $n = \log(d)$) depending on the structure of the circuit. By applying these random unitaries to a fixed input state and measuring in the computational basis, one obtains a probability distribution on measurement outcomes, from which it may be hard to sample using a classical device.

For hardness of classical sampling, we want the probability distribution on measurement outcomes to be *anticoncentrated*.¹ A sufficient condition for this is that the unitary produced by the circuit is sufficiently close to the uniform distribution: namely, that it is a *unitary 2-design*. We now explain what this means. Given any measure dU on $U(d)$, the k -th moments $M_k(dU)$ of dU are defined by

$$\int_{U(n)} dU U_{i_1, j_1} \cdots U_{i_k, j_k} \overline{U_{i'_1, j'_1}} \cdots \overline{U_{i'_k, j'_k}},$$

where $U_{i,j}$ is the (i, j) -th entry of the matrix U , and the bar signifies complex conjugation. When the measure is the Haar measure² dU_H , these moments

¹We don't need to worry about what this means here, but see e.g. [1].

²The Haar measure is the uniform (translationally invariant) measure on $U(d)$.

are given by the so-called *Weingarten functions* [4]. The first and second moments have a straightforward expression:

$$M_1(dU_H) = \int_{U(n)} dU_H U_{i_1, j_1} \overline{U_{i'_1, j'_1}} = \frac{1}{d} \delta_{i_1 i'_1} \delta_{j_1 j'_1} \quad (1)$$

$$\begin{aligned} M_2(dU_H) &= \int_{U(n)} dU_H U_{i_1, j_1} U_{i_2, j_2} \overline{U_{i'_1, j'_1}} \overline{U_{i'_2, j'_2}} \\ &= \frac{1}{d^2 - 1} (\delta_{i_1 i'_1} \delta_{i_2 i'_2} \delta_{j_1 j'_1} \delta_{j_2 j'_2} + \delta_{i_1 i'_2} \delta_{i_2 i'_1} \delta_{j_1 j'_2} \delta_{j_2 j'_1}) \\ &\quad - \frac{1}{d(d^2 - 1)} (\delta_{i_1 i'_1} \delta_{i_2 i'_2} \delta_{j_1 j'_2} \delta_{j_2 j'_1} + \delta_{i_1 i'_2} \delta_{i_2 i'_1} \delta_{j_1 j'_1} \delta_{j_2 j'_2}) \quad (2) \end{aligned}$$

We say that a measure dU is a unitary 2-design precisely when it has the same first and second moments as dU_H , that is:

$$M_1(dU) = M_1(dU_H) \quad M_2(dU) = M_2(dU_H)$$

Is it possible to create an efficient parametrised random circuit family that induces a unitary 2-design? It seems so, following a paper presented by Saeed Mehraban at QIP this year [2]. With Harrow, Mehraban showed that short-depth random circuits involving nearest-neighbour unitary gates (where proximity is defined by a cubic lattice structure) produce approximate unitary t -designs. This is precisely the experimental model of Google's Quantum AI group, who are considering a 49-qubit 2-dimensional lattice of qubits. It seems that randomised quantum circuits inducing 2-designs on the unitary group may be available in the near future.

We have already discussed the application of such circuits to demonstrate quantum supremacy. But, can we use them to do anything computationally useful? Here we will discuss a possible application to finding the ground state of a Hamiltonian.

Variational quantum eigensolvers. A common problem in quantum chemistry, quantum neural networks, and elsewhere, is to find the *ground state* or *ground energy* of a given Hamiltonian H on n qubits. Recall that, for $|\psi\rangle$ a quantum state of n qubits, the energy of $|\psi\rangle$ is defined as $\langle \psi | H | \psi \rangle$. The ground state $|\psi_0\rangle$ of H minimises this quantity, and its energy is called the ground energy.

Obviously, this can be thought of as a minimisation problem over $U(d)$: since $|\psi\rangle$ can be expressed as $U|0\rangle$ for some U , let $f_H(U) = \langle 0 | U^\dagger H U | 0 \rangle$,

and our problem becomes the problem of finding

$$\min_{U \in U(d)} f_H(U).$$

We might try a variational approach. Suppose that we indeed have a parametrised circuit family inducing a distribution on $U(d)$ which is roughly uniform (say, a unitary 2-design). We can use the circuit to generate a random unitary in $U(d)$. Then, varying our parameters, we can find the direction in parameter space in which f_H is decreasing fastest. Moving in this direction, we will arrive at a local minimum. Iterating this procedure, we will (with some assumptions on H) hopefully eventually find the global minimum with some high probability.

An important difficulty with this approach is the problem of *barren plateaus*.

Barren plateaus. Roughly, this problem is as follows:

Let H be a Hamiltonian on n qubits, and let the measure dU on $U(d)$, where $d = 2^n$, be a unitary 2-design. If a random unitary U is picked according to this measure, the expected gradient of f_H in any direction is zero, and the variance is damped exponentially with respect to qubit number n .

Clearly, this is an important consideration for the variational approach with large numbers of qubits, where one picks a unitary uniformly at random: with high probability, one will choose a random unitary on a *barren plateau*, where the change in f_H in any direction is nearly zero. Since it is intuitively obvious that the gradient descent approach works fastest when the gradient is steepest, this problem could make the approach inefficient.

Let us now state the theorem formally, and then prove it. For clarity, we recall some facts about the unitary group. The unitary group $U(d)$ is a Lie group, a group which is also a manifold: a neighbourhood of every element $U \in U(d)$ can be identified smoothly with a real vector space (in this case, \mathbb{R}^{d^2}). Just as for \mathbb{R}^{d^2} , the space of possible directions in which one can move from each point in $U \in U(n)$ is a d^2 -dimensional real vector space, called the *tangent space* T_U . For any function $f : U(n) \rightarrow \mathbb{C}$, each direction $A \in T_U$ defines a derivative $(df/dA)_U$ giving the change in the function along that direction.

As a Lie group, $U(d)$ has a privileged tangent space — the tangent space of the identity $\mathbb{1} \in U(d)$. This tangent space $T_{\mathbb{1}} = \mathfrak{u}(d)$ has additional

structure (which we will not use here) and is known as the *Lie algebra* of $U(d)$. The fact we will use is that a basis for $\mathfrak{u}(d)$ gives us a canonical basis for T_U , for every U , as follows. Since multiplication in a Lie group is a diffeomorphism, it induces isomorphisms of tangent spaces. Given a vector in $\mathfrak{u}(d)$, one therefore obtains a vector in T_U for any $U \in U(d)$ using the isomorphism $T_{\mathbb{1}} \rightarrow T_U$ induced by left multiplication by U . This therefore associates to each element of $\mathfrak{u}(d)$ a smoothly varying field of directions in T_U , for every U , called a *left-invariant vector field*.

The point of all this is that it allows us to define any curve through a general point in $U(d)$ in terms of an element of the Lie algebra $\mathfrak{u}(d)$. Since $U(d)$ is a matrix Lie group, we can obtain concrete expressions:

- $\mathfrak{u}(d)$ is the vector space of $d \times d$ antihermitian matrices.
- The gradient $(\frac{df}{dA})_U$ of the smooth function $f : U(d) \rightarrow \mathbb{C}$ at the point U along the direction given by the left-invariant vector field of $A \in \mathfrak{u}(d)$ is

$$\frac{d}{dt} f(Ue^{tA})|_{t=0}, \quad (3)$$

where e^{tA} is the matrix exponential.

We can now state the theorem.

Theorem 0.1. *Let H be some Hamiltonian on $n = \log(d)$ qubits, let $f_H : U(d) \rightarrow \mathbb{C}$ be the energy function, and let dU be some measure on $U(d)$ which is a unitary 2-design. Then for any $A \in \mathfrak{u}(d)$, we have*

$$\mathbb{E}[(\frac{df}{dA})_U] = 0 \quad (4)$$

$$\text{Var}[(\frac{df}{dA})_U] = \frac{2((AA^\dagger)_{00} - |(A)_{00}|^2)}{d^2 - 1} (\text{Tr}(HH^\dagger) - \frac{1}{d} |\text{Tr}(H)|^2) \quad (5)$$

where the expectation and variance are taken over $U \in U(n)$, with respect to the measure dU .

Clearly, the fact that the expectation is zero and the variance decreases exponentially with n shows that the gradient tends to zero everywhere. Before proving the theorem, it's worth making some reassuring noises — this doesn't mean our 2-design circuits are useless. Firstly, the gradient is only everywhere zero in the limit $n \rightarrow \infty$; in general, this is just information that

will help us estimate how fast the gradient descent will approach a minimum, and there is no reason why, for H such that $\text{Tr}(HH^\dagger)$ is large, the variational approach using a 2-design may not still be useful. Secondly, this theorem only applies to gradient descent approaches; ‘hopping’ approaches might avoid this problem, although then one would not obviously be able to take advantage of the smoothness of f_H . Finally, this theorem depends on a uniformly random choice of unitary; if one knows something about where the non-barren areas are, one can try to pick a probability measure which hits those areas.

We now give the proof, which is somewhat simpler than that in [3], since we do not worry about circuit parametrisations.

Proof. We first calculate $(\frac{df}{dA})_U$ using (3). Note first of all that, for any curve $x(t) \in U(n)$, since $x^\dagger(t)x(t) = \mathbb{1}$ it follows by the product rule that $\frac{dx^\dagger}{dt} = -x^\dagger \frac{dx}{dt} x^\dagger$. Let $x(t) = Ue^{tA}$; clearly $\frac{dx}{dt} = UAe^{tA}$. Then we have

$$\begin{aligned} \frac{d}{dt} \langle 0 | x^\dagger H x | 0 \rangle |_{t=0} &= \langle 0 | -AU^\dagger H U + U^\dagger H U A | 0 \rangle \\ &= \langle 0 | [U^\dagger H U, A] | 0 \rangle. \end{aligned} \tag{6}$$

We now want to evaluate the expectation (4)

$$\mathbb{E}[(\frac{df}{dA})_U] \stackrel{(6)}{=} \langle 0 | \left(\int dU [U^\dagger H U, A] \right) | 0 \rangle. \tag{7}$$

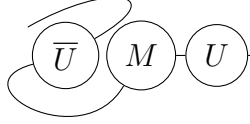
For this we use the fact that dU is a unitary 1-design. To see how (1) relates to (7), consider the matrix entries of the integral:

$$\begin{aligned} \left(\int dU U^\dagger M U \right)_{i,l} &= \sum_{j,k} \int dU \overline{U_{j,i}} M_{j,k} U_{k,l} \stackrel{(1)}{=} \frac{1}{d} \sum_{j,k} \delta_{j,k} \delta_{i,l} M_{j,k} = \frac{\text{Tr}(M)}{d} \delta_{i,l} \\ &\Rightarrow \int dU U^\dagger M U = \frac{\text{Tr}(M)}{d} \mathbb{1} \end{aligned} \tag{8}$$

We immediately see that (7) vanishes, since the commutator of anything with the identity is zero. Therefore (4) is proved.

We note before moving on to prove (5) that the unitary 1-design equation (1) just gives information about index identification. There is a neat diagrammatic notation for this. Write the matrices in the integrand as nodes,

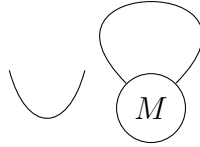
joined with wires corresponding to indices. For instance, $U^\dagger M U$ is written as



Now the rule (1) just says:

Remove the \bar{U} and U nodes, connecting the left wire of \bar{U} to the left wire of U and the right wire of \bar{U} to the right wire of U , and multiply by $\frac{1}{d}$.

Doing this we get $\frac{1}{d}$ multiplied by the diagram

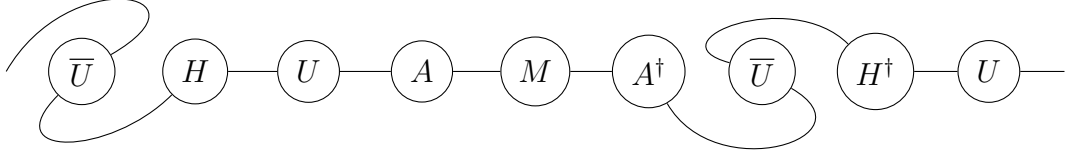


which is precisely $\text{Tr}(M)\mathbb{1}$. (The cup is the identity, as you can check by plugging it into anything, and the loop is the trace.) We therefore recover the derivation (8).

These diagrams help a lot in calculating the variance. Here we have (letting $M := |0\rangle\langle 0|$):

$$\begin{aligned} \text{Var} \left[\left(\frac{df}{dA} \right)_U \right] &= \mathbb{E} \left[\left| \left(\frac{df}{dA} \right)_U \right|^2 \right] \\ &= \langle 0| \int dU U^\dagger H U A M A^\dagger U^\dagger H^\dagger U + \int dU A U^\dagger H U M U^\dagger H^\dagger U A \\ &\quad - \int dU A U^\dagger H U M A^\dagger U^\dagger H^\dagger U - \int dU U^\dagger H U A M U^\dagger H^\dagger U A^\dagger |0\rangle \end{aligned} \tag{9}$$

I will evaluate the first of the four integrals as an example, then leave the others for the reader. The diagram for the integrand is



Now we have two U 's (call them U_1, U_2 from L to R) and two \bar{U} 's (call them \bar{U}_1, \bar{U}_2 from L to R) and can use the equation for the second moment of a 2-design (2). In words, remove these and:

$$\frac{1}{d^2 - 1} \left(\left\{ \begin{array}{l} \text{connect L-L and} \\ \text{R-R of the pairs} \\ (U_1, \bar{U}_1) \quad \text{and} \\ (U_2, \bar{U}_2) \end{array} \right\} + \left\{ \begin{array}{l} \text{connect L-L and} \\ \text{R-R of the pairs} \\ (U_1, \bar{U}_2) \quad \text{and} \\ (U_2, \bar{U}_1) \end{array} \right\} \right)$$

$$-\frac{1}{d(d^2 - 1)} \left(\left\{ \begin{array}{l} \text{connect L-L} \\ \text{of the pairs} \\ (U_1, \bar{U}_1) \quad \text{and} \\ (U_2, \bar{U}_2) \quad \text{and} \\ \text{R-R of the pairs} \\ (U_1, \bar{U}_2) \quad \text{and} \\ (U_2, \bar{U}_1) \end{array} \right\} + \left\{ \begin{array}{l} \text{connect R-R} \\ \text{of the pairs} \\ (U_1, \bar{U}_1) \quad \text{and} \\ (U_2, \bar{U}_2) \quad \text{and} \\ \text{L-L of the pairs} \\ (U_1, \bar{U}_2) \quad \text{and} \\ (U_2, \bar{U}_1) \end{array} \right\} \right)$$

The resulting diagrammatic expression is

$$\begin{aligned}
& \frac{1}{d^2 - 1} \left(\begin{array}{c} \text{Diagram 1} \\ + \\ \text{Diagram 2} \end{array} \right) \\
& - \frac{1}{d(d^2 - 1)} \left(\begin{array}{c} \text{Diagram 3} \\ + \\ \text{Diagram 4} \end{array} \right)
\end{aligned}$$

This evaluates as

$$\begin{aligned}
X & := \frac{1}{d^2 - 1} (|\text{Tr}(H)|^2 AMA^\dagger + \text{Tr}(HH^\dagger)\text{Tr}(AMA^\dagger)\mathbb{1}) \\
& - \frac{1}{d(d^2 - 1)} (|\text{Tr}(H)|^2\text{Tr}(AMA^\dagger)\mathbb{1} + \text{Tr}(HH^\dagger)AMA^\dagger).
\end{aligned}$$

Given $M = |0\rangle\langle 0|$, we obtain

$$\begin{aligned}
\langle 0|X|0\rangle & = \frac{1}{d^2 - 1} (|\text{Tr}(H)|^2|A_{00}|^2 + \text{Tr}(HH^\dagger)(A^\dagger A)_{00}) \\
& - \frac{1}{d(d^2 - 1)} (|\text{Tr}(H)|^2(A^\dagger A)_{00} + \text{Tr}(HH^\dagger)|A_{00}|^2).
\end{aligned}$$

Doing the same for all the terms in (9) and totalling up, the reader can easily check that (5) holds.

References

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