Connecting ansatz expressibility to gradient magnitudes and barren plateaus

Zoë Holmes,1 Kunal Sharma,2,3 M. Cerezo,3,4 and Patrick J. Coles3

1Information Sciences, Los Alamos National Laboratory, Los Alamos, NM, USA.
2Hearne Institute for Theoretical Physics, Department of Physics and Astronomy, and Center for Computation and Technology, Louisiana State University, Baton Rouge, Louisiana 70803, USA.
3Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA.
4Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos, NM, USA.

Parameterized quantum circuits serve as ansätze for solving variational problems and provide a flexible paradigm for programming near-term quantum computers. Ideally, such ansätze should be highly expressive so that a close approximation of the desired solution can be accessed. On the other hand, the ansatz must also have sufficiently large gradients to allow for training. Here, we derive a fundamental relationship between these two essential properties: expressibility and trainability. This is done by extending the well established barren plateau phenomenon, which holds for ansätze that form exact 2-designs, to arbitrary ansätze. Specifically, we calculate the variance in the cost gradient in terms of the expressibility of the ansatz, as measured by its distance from being a 2-design. Our resulting bounds indicate that highly expressive ansätze exhibit flatter cost landscapes and therefore will be harder to train. Furthermore, we provide numerics illustrating the effect of expressibility on gradient scalings, and we discuss the implications for designing strategies to avoid barren plateaus.

I. Introduction

While quantum hardware is rapidly reaching the stage where it can outperform classical supercomputers [1], we remain in the Noisy Intermediate-Scale Quantum (NISQ) era in which the available devices are relatively small and prone to errors [2]. Variational quantum algorithms have gathered attention as a computational strategy that is well suited to the constraints imposed by NISQ devices [3–20]. In VQAs a problem-specific cost function is efficiently evaluated on a quantum computer, while a classical optimizer trains a parameterized quantum circuit to minimize this cost. The benefit of this paradigm is that it adapts to the qubit and connectivity constraints of NISQ devices, while keeping the circuit depth short to mitigate quantum hardware noise.

Central to the success of VQAs is the construction of a parameterized quantum circuit, which serves as an ansatz with which to explore the space of solutions to the target problem. Some noteworthy ansätze include the quantum alternating operator ansatz [5, 21], coupled cluster ansatz [22–24], Hamiltonian variational ansatz [25], and hardware efficient ansatz [26]. To successfully find an optimal solution, the ansatz must be both expressive and trainable. Specifically, the ansatz must be sufficiently expressive such that it contains a circuit that well-approximates the optimal solution. Concurrently, the cost landscape must be sufficiently featured to be able to train the parameters to find this optimal solution.

Recently, it was shown that VQAs can exhibit barren plateaus, where under certain conditions the gradient of the cost function vanishes exponentially with the size of the system [27–36]. In particular, Ref. [27] demonstrated that if an ansatz is sufficiently random that it matches the uniform distribution of unitaries up to the second moment (i.e., forms a 2-design), then the variance in the cost gradient will vanish exponentially with the number of qubits. Several strategies have been proposed to address this issue [37–46], such as clever parameter initialization or ansatz construction, while more research is needed to test these strategies on various problems.

In broad terms, the expressibility of an ansatz is determined by how uniformly it explores the unitary space. Thus the distance between the distribution of unitaries generated by an ansatz and the maximally expressive uniform distribution of unitaries is a natural measure of its expressibility [47]. Using such a measure, Ref. [48] calculated the expressibility for several commonly used ansätze and, by using the cost gradients obtained in [28], suggested that in some cases it is possible for an ansatz to be both expressive and trainable. Additionally, Ref. [49] noted a numerical correlation between expressibility and trainability for analog systems. However, given that both expressibility and trainability are closely related to randomness, one might expect to be able to draw a more fundamental and general relationship between expressibility and trainability.

Here we demonstrate that this is indeed the case by analytically relating the trainability of an ansatz to its expressibility. This is done by extending the barren plateau phenomenon introduced in [27], which holds for ansätze that form exact 2-designs, to arbitrary ansätze. Specifically, we upper bound the variance in the cost gradient in terms of the distance the ansatz is from being a 2-design. Since the degree to which an ansatz is a 2-design is a measure of its expressibility, this allows us to relate the gradient of the cost landscape to the expressibility of the ansatz. We find that the more expressive the ansatz, the smaller the variance in the cost gradient and hence the flatter the landscape.

Our main results can be summarized in Fig. 1. Given an ansatz, we analyze the space of unitaries accessible when sampling the parameters (Fig. 1(A)) of a parametrized quantum circuit. Inexpressive ansätze,
such as the one shown in Fig. 1(B), access a small region of the unitary group and can include the space of unitaries that solve certain problems but not the space that solve others. Our results do not preclude inexpressive ans"{a}tze having trainability issues, such as barren plateaus. On the other hand, highly expressive ans"{a}tze, which are generically used for many problems as they can access a much larger space (Fig. 1(C)), are shown to lead to small gradients, and hence can have trainability issues.

Since our analytic bounds are upper bounds, they leave open the questions of how reducing the expressibility of an ansatz changes the cost landscape, and hence how reducing the expressibility can be avoided without the barren plateau phenomenon. To address these questions we provide extensive numerics studying the effect that tuning the expressibility of an ansatz may have on the scaling of gradient magnitudes. Specifically, we consider the effects of decreasing the depth of the circuits, correlating circuit parameters, and restricting either the direction or angle of rotations. We find that strongly correlating parameters [37] and/or initializing close to the solution (and then restricting the ansatz to explore the region close to the initialization [38]) to be the most effective approaches to avoid exponentially vanishing cost gradients.

II. Preliminaries

A. General framework

Variational Quantum Algorithms (VQAs) encode an optimization task in a cost function whose minimum corresponds to the solution of the problem. Here we consider cost functions of the form\(^1\)

\[ C_{p,H}(\theta) = \text{Tr}[H U(\theta) \rho U(\theta)\dagger], \]  

(1)

where \(\rho\) is an \(n\)-qubit input state, \(H\) is a Hermitian operator, and \(U(\theta)\) is a parametrized quantum circuit depending on trainable parameters \(\theta\). The value of the cost \(C_{p,H}(\theta)\) (or of its gradient) are estimated on a quantum computer, and then are fed into a classical optimizer which attempts to solve the optimization task \(\text{arg min}_\theta C_{p,H}(\theta)\).

The success of the VQA hinges on several factors. First, it is necessary to find an operator \(H\) such that the resulting cost is faithful for the given problem. That is, we require the minimum of \(C_{p,H}(\theta)\) to correspond to the solution of the optimization task. Evidently, for some applications, there may be multiple choices in \(H\) corresponding to faithful costs and therefore other factors will determine which to use. One such factor is how easily \(H\) can be measured on a quantum computer. Another relevant feature, as discussed further in Section IID, is the locality of \(H\), i.e., the number of qubits it acts non-trivially on. We say that the cost function is global if \(H\) acts non-trivially on all qubits, while we use the term \(k\)-local for costs where \(H\) acts non-trivially on at most \(k\) qubits.

A second aspect that determines the success of a VQA is the choice in ansatz for \(U(\theta)\). While discrete parameterizations are possible, usually \(\theta\) are continuous parameters, such as gate rotation angles, in a parametrized quantum circuit. Generally, \(U(\theta)\) is expressed as

\[ U(\theta) = \prod_{j=1}^{D} U_j(\theta_j) W_j. \]  

(2)

\(^1\)In Appendix D we extend our results to more general costs of the form \(C_{\text{gen}} = \sum_{i,j} \text{Tr}[H_i U(\theta) \rho_i U(\theta)\dagger]\). This cost allows for multiple input states \(\rho_i\) and measurement operators \(H_i\), opening up quantum machine learning approaches that employ training data [50–53].
Here \( \{ W_j \}_{j=1}^{N} \) is a chosen set of fixed unitaries and \( U_j = e^{-i \theta_j} V_j \) is a rotation of angle \( \theta_j \), generated by a Hermitian operator \( V_j \) such that \( (V_j)^2 = 1 \). The rotation angles \( \{ \theta_j \} \) are typically assumed to be independent.

Once an ansatz has been fixed for the parametrized quantum circuit, then, as sketched in Fig. 1(A), each possible vector of parameters \( \theta \) corresponds to a unitary \( U(\theta) \) that is produced. For concreteness, given a set of different parameters \( \{ \theta^{(1)}, \theta^{(2)}, ..., \theta^{(v)} \} \) we obtain the corresponding ensemble of unitaries

\[
\mathcal{U} = \{ U^{(1)}, U^{(2)}, ..., U^{(v)} \},
\]

where \( U^{(j)} := U(\theta^{(j)}) \). Here, \( \mathcal{U} \subseteq \mathcal{U}(d) \), where \( \mathcal{U}(d) \) is the unitary group \( \mathcal{U}(d) \) of degree \( d = 2^n \).

### B. Expressibility

For a VQA to be successful, a solution (i.e., a unitary which is by some measure close to the unitary that minimizes the cost) needs to be contained within the ensemble of unitaries generated by the ansatz. Specifically, defining \( \mathcal{U}_a \) as the set of solution unitaries, then the VQA will be successful only if \( \mathcal{U}_a \cap \mathcal{U} \neq \emptyset \). When this condition is satisfied the ansatz is said to be complete for the given problem.

In the absence of prior knowledge about where the solution unitaries \( \mathcal{U}_a \) lie, the likelihood that the ansatz is complete can be maximized by using an ansatz that explores the total space of unitaries as fully and as uniformly as possible. Such ansätze are known as expressive ansätze. For example, consider having two problems (problem \( A \) and problem \( B \)), with solution spaces respectively denoted as \( \mathcal{U}_a^A \) and \( \mathcal{U}_a^B \). Figure 1(B) sketches \( \mathcal{U} \) for an insufficient ansatz which is complete with respect to problem \( A \) but incomplete with respect to \( B \). Conversely, Fig. 1(C) shows \( \mathcal{U} \) for an expressive ansatz which is complete with respect to both problems.

For many applications, information about the problem can be encoded in the ansatz. For instance, the quantum alternating operator ansatz [21] (or the Hamiltonian variational ansatz [25]), encode information of an appropriate adiabatic transformation. Such problem-inspired ansätze may be complete but inexpressive (e.g., Fig. 1(B) could denote a problem-inspired ansatz for problem \( A \)). However, problem-agnostic ansätze, which can be used for a wide range of problems, need to be sufficiently expressive to guarantee their completeness.

The expressibility of an ansatz, i.e., the degree to which it uniformly explores the unitary group \( \mathcal{U}(d) \), can be quantified by comparing the uniform distribution of unitaries obtained from the ensemble \( \mathcal{U} \) to the maximally expressive uniform (Haar) distribution of unitaries from \( \mathcal{U}(d) \). More concretely, the expressibility of a circuit can be defined in terms of the following super-operator [47, 48]:

\[
\mathcal{A}_U^{(t)}(\cdot) := \int_{\mathcal{U}(d)} d\mu(V) V^\otimes t (\cdot) (V^\dagger)^\otimes t - \int_{\mathcal{U}} dU U^\otimes t (\cdot) (U^\dagger)^\otimes t,
\]

where \( d\mu(V) \) is the volume element of the Haar measure and \( dU \) is the volume element corresponding to the uniform distribution over \( \mathcal{U} \) in Eq. (3). If \( \mathcal{A}_U^{(t)}(X) = 0 \) for all operators \( X \), then averaging over elements of \( \mathcal{U} \) agrees with averaging over elements of the Haar distribution over \( \mathcal{U}(d) \) up to the \( t \)-th moment, and thus \( \mathcal{U} \) forms a \( t \)-design [54–58]. For our purposes it suffices to consider the behavior of \( \mathcal{A}_U^{(t)} \) for \( t = 2 \). Henceforth we drop the \( t \)-superscript, i.e., \( \mathcal{A}_U = \mathcal{A}_U^{(2)} \).

In the context of minimizing a generic cost \( C_{p,H}(\theta) \) of the form specified by Eq. (1), we are interested in the expressibility of the circuit with respect to both the initial state \( \rho \) and the measurement operator \( H \). The following quantities respectively capture these notions:

\[
\varepsilon_U^p := ||A_U(\rho^\otimes 2)||_2 \quad (5)
\]

\[
\varepsilon_U^H := ||A_U(H^\otimes 2)||_2 \quad (6)
\]

Small values of \( \varepsilon_U^p \) and \( \varepsilon_U^H \) indicate that the ansatz is highly expressive. These measures generalize the notion of expressibility introduced in [47] where the expressibility was defined in terms of \( \varepsilon_U^p \) for \( \rho = |0\rangle \langle 0| \).

While the \( \rho \) and \( H \) dependence of \( \varepsilon_U^p \) and \( \varepsilon_U^H \) make them natural measures of the expressibility in the context of minimizing a cost \( C_{p,H}(\theta) \), cost function-independent measures of expressibility may allow the expected performance of different ansätze to be more easily compared. With this in mind, one could alternatively quantify the expressibility directly in terms of the diamond norm of \( \mathcal{A}_U \),

\[
\varepsilon_U^\diamond := ||\mathcal{A}_U||_\diamond, \quad (7)
\]

which is an operationally meaningful distance measure to distinguish two quantum operations. We use the diamond norm here in line with the literature on \( \varepsilon \)-approximate unitary designs [59]; however, alternative norms can be used (for a discussion, see [57]). For completeness we will formulate our results in terms of \( \varepsilon_U^\diamond \), as well as the quantities \( \varepsilon_U^p \) and \( \varepsilon_U^H \).

### C. Gradient Magnitudes

For a variational quantum algorithm to run successfully it is not sufficient that the ansatz contains the solution; the cost landscape must also exhibit large enough cost gradients to enable this solution to be found.

The component of the gradient corresponding to the parameter \( \theta_k \) is determined by the partial derivative
\[ \partial_k C := \frac{\partial C_{\theta_k}}{\partial \theta_k}. \]

For a generic ansatz of the form specified by Eq. (2), the average of \( \partial_k C \) over all parameters \( \theta \) vanishes

\[ \langle \partial_k C \rangle = 0 \quad \forall \; k. \quad (8) \]

That is, the cost gradients are not biased in any single direction but rather average out to zero. Intuitively, this lack of bias can be understood as following from the fact that the average of a rotation \( \exp(-i\theta_k V_k) \) is zero when \( V_k^2 = 1 \). We show this in Appendix C, where we prove that \( \langle \partial_k C \rangle = 0 \) by explicitly integrating over \( \theta_k \).

However, an unbiased cost landscape can be either trainable or untrainable, depending on the extent to which the gradient fluctuates away from zero. Therefore, to assess the trainability of an ansatz \( U(\theta) \), we now recall Chebyshev’s inequality. This inequality bounds the probability that the partial derivative of the cost deviates from its average of zero,

\[ P(|\partial_k C| \geq \delta) \leq \frac{\text{Var}[\partial_k C]}{\delta^2}, \quad (9) \]

in terms of the variance

\[ \text{Var}[\partial_k C] = \left\langle (\partial_k C)^2 \right\rangle - \langle \partial_k C \rangle^2, \quad (10) \]

where the expectation value is taken over the parameters \( \theta \). Hence if the variance of the partial derivative is small for all \( \theta_k \), then the probability that the partial derivative is non-zero is small for all \( \theta_k \). On such landscapes, (potentially untenably) precise measurements are required to detect the path of steepest descent to navigate to the minimum.

D. Barren Plateaus

There is a growing awareness of the so called barren plateau phenomenon for variational quantum algorithms [27–36]. For a given ansatz \( U(\theta) \), a cost \( C \) is said to exhibit a barren plateau if its gradients vanish exponentially with the number of qubits \( n \). This is typically relaxed to a probabilistic definition, where the gradient vanishes exponentially with high probability. This would follow from Chebyshev’s inequality, Eq. (9), if the variance in the partial derivative vanishes exponentially, i.e., if \( \text{Var}[\partial_k C] \in \mathcal{O}(2^{-pn}) \) for any integer \( p > 0 \). For costs that exhibit barren plateaus, exponentially precise measurements may be required to determine the minimization direction, and hence the cost is effectively untrainable for large problem sizes.

To elucidate the conditions under which a layered parameterized ansatz \( U(\theta) \), of the form of Eq. (2), gives rise to barren plateaus, consider a bipartite cut of \( U(\theta) \) and write

\[ U(\theta) = U_L(\theta)U_R(\theta) \quad (11) \]

where

\[ U_L(\theta) = \prod_{j=k+1}^{D} U_j(\theta_j)W_j \quad \text{and} \quad U_R(\theta) = \prod_{j=1}^{k} U_j(\theta_j)W_j. \quad (12) \]

Note that since we suppose the parameters \( \theta_j \) are uncorrelated, the circuits \( U_L \) and \( U_R \) are independent.

Ref. [27] then demonstrated that if the ensemble of unitaries generated by the ansatz \( U(\theta) \) is sufficiently random (i.e., expressive) such that the ensembles \( U_L \) or \( U_R \) (associated with the circuits \( U_L(\theta) \) and \( U_R(\theta) \) respectively) form a 2-design, then the variance in the cost gradient vanishes exponentially with \( n \). Specifically, let us denote the variance of the cost when just \( U_R \), just \( U_L \), and both \( U_R \) and \( U_L \) form 2-designs as \( \text{Var}_R\partial_k C \), \( \text{Var}_L\partial_k C \), and \( \text{Var}_{R,L}\partial_k C \), respectively. From Ref. [27] it follows that for \( x = R, L \) and \( x = R, L \),

\[ \text{Var}_x\partial_k C = \frac{g_x(p, H, U)}{2^{2n} - 1}, \quad (13) \]

where we have pulled out the \( n \)-dependent scaling factor explicitly. The prefactor \( g_x(p, H, U) \), which we define explicitly in Appendix E, is in \( \mathcal{O}(2^n) \) for typical choices in \( V_k \) and \( H \). Thus if \( U_L \) or \( U_R \) form a 2-design, the variance in the gradient vanishes exponentially in \( n \). In other words, maximally expressive ansätze exhibit barren plateaus.

III. Main Results

A. Analytic Bounds

In this section, we study the gradient of a generic cost \( C_{\rho, H}(\theta) \), Eq. (1), with an ansatz \( U(\theta) \), Eq. (2), but relax the assumption that \( U_R \) or \( U_L \) forms a 2-design. By doing so, we extend the results on barren plateaus from Ref. [27] to arbitrary ansätze. As will become clear, this generalization enables us to relate the variance of the cost function partial derivative to the expressibility of \( U(\theta) \) in Eq. (4).

Let us start by noting that while maximally expressive ansätze exhibit barren plateaus, the converse is not necessarily true. In other words, highly inexpressive ansätze need not always experience large cost gradients, and in fact they may exhibit vanishing gradients. A trivial example of this phenomenon is provided by an ansatz composed of rotations that commute with the measurement operator \( [U(\theta), H] = 0 \). Such an ansatz will leave the cost unchanged for any \( \theta \) and so the variance in gradient in the cost of such an ansatz is necessarily zero. A more subtle example is an ansatz composed of a tensor product of single qubit rotations. Since this ansatz does not generate entanglement it is inexpressive; however, it has also been shown to exhibit a barren plateau for global cost functions [7, 28]. It follows from these observations
that it is not possible to meaningfully lower bound the gradients of an ansatz in terms of its expressibility.

Therefore to relate cost gradients to expressibility we instead derive an upper bound. Specifically, our main result consists of a non-trivial upper bound for the variance of the cost function partial derivative for a general ansatz $U(\theta)$ in terms of the expressibility in (4). This bound is in terms of: (1) the variance of the cost gradient when either $U_L$ or $U_R$ form a 2-design, and (2) the expressibility of the ansatz as measured by the distance $\rho$ between $U_L$ and $U_R$ are from being 2-designs. As shown in Appendix D, we prove the following.

**Theorem 1.** Consider a generic cost function $C_{\rho,H}(\theta)$, Eq. (1), using a layered ansatz $U(\theta)$ of the general form in Eq. (2). The variance of the cost partial derivative obeys the following bounds:

\[
\begin{align*}
\text{Var}_\theta C &\leq \text{Var}_R \partial_\theta C + 4\varepsilon^R \| H \|_2^2, \\
\text{Var}_\theta C &\leq \text{Var}_L \partial_\theta C + 4\varepsilon^L \| \rho \|_2^2, \\
\text{Var}_\theta C &\leq \text{Var}_{R,L} \partial_\theta C + f(\varepsilon^L, \varepsilon^R).
\end{align*}
\]

Here we used the shorthand $\varepsilon^R := \varepsilon^R_{U_R}$ and $\varepsilon^L := \varepsilon^L_{U_L}$, and we have defined

\[
f(x,y) := 4\varepsilon^R \varepsilon^L + \frac{2^{n+2} (x\| H \|_2^2 + y\| \rho \|_2^2)}{2^{2n} - 1}.
\]

Theorem 1 establishes a formal relationship between the gradient of the cost landscape and the expressibility of the ansatz used. Namely, the higher the expressibility of the ansatz, that is the smaller $\varepsilon^H$ or $\varepsilon^R$, the smaller the upper bound on the variance of the cost partial derivative. This, in combination with the fact that the cost gradient is unbiased, demonstrates that highly expressive ansätze will have flatter landscapes and consequently be harder to train.

It is important to stress that, in contrast to the bounds specified by Eqs. (13), the bounds in Eqs. (14)–(16) do not correspond to three different choices in ansatz but rather hold for any ansatz of the form in Eq. (2). Thus any single bound would suffice to bound the variance in the cost function partial derivative. We include all three bounds despite this fact since in any instance one bound may be tighter than the others and hence more informative.

In Appendix D, we extend Theorem 1 to cost functions of the form $C_{\text{gen}} = \sum_i \text{Tr}[H_i U(\theta) \rho_i U(\theta)]$, which allow for multiple input states and measurements. Thus our results also apply to quantum machine learning approaches that utilize training data.

**Generalizing the Barren Plateau phenomenon.** Theorem 1 may be viewed as an extension of the barren plateau phenomenon introduced in Ref. [27] to ansätze that form approximate, rather, than exact 2-designs. By combining Eq. (13) and Eq. (16), we find that the variance in the partial derivative for an arbitrary ansatz is bounded as

\[
\text{Var}_\theta C \leq \frac{g_{L,R}(\rho, H, U)}{2^{2n} - 1} + f(\varepsilon^L, \varepsilon^R).
\]

Here the first term on the right is the variance of a maximally expressive ansatz (namely, one that forms a 2-design) and $f(\varepsilon^L, \varepsilon^R)$ is the expressibility dependent correction term defined in Eq. (17). Expressions similar to Eq. (18) are obtainable from Eq. (14) and Eq. (15).

For perfectly expressive ansätze, $f(\varepsilon^L, \varepsilon^R)$ vanishes and Eq. (18) reduces to Eq. (13), regaining the result of Ref. [27]. In this case, the variance in the gradient vanishes exponentially with the size of the system $n$, i.e., the ansatz exhibits a barren plateau. Similarly, if the expressibility of an ansatz increases exponentially with the size of the problem, i.e., if $f(\varepsilon^L, \varepsilon^R) \in \mathcal{O}(\frac{1}{2^n})$ for $k > 0$, then $\text{Var}_\theta C$ again vanishes exponentially and the ansatz exhibits a barren plateau. However, more generally, when $f(\varepsilon^L, \varepsilon^R)$ scales non-exponentially the upper bound allows for the variance in the partial derivative to be non-vanishing. Thus, there is leeway for imperfectly expressive ansätze to avoid barren plateaus.

**Diamond Norm Reformulation.** For local costs the term $\| H \|_2^2$ scales exponentially with the size of the system and therefore for large systems (14) becomes exponentially loose. This issue can be mitigated by reformulating Theorem 1 in terms of $\varepsilon^L_{\theta}$, Eq. (7). We obtain the following theorem in Appendix D.

**Theorem 2.** Consider a generic cost function $C_{\rho,H}(\theta)$, Eq. (1), using a layered ansatz $U(\theta)$ of the general form in Eq. (2). The variance of the cost partial derivative obeys the following bounds:

\[
\begin{align*}
\text{Var}_\theta C &\leq \text{Var}_R \partial_\theta C + 4\| H \|_\infty^2 \varepsilon^R, \\
\text{Var}_\theta C &\leq \text{Var}_L \partial_\theta C + 4\| \rho \|_\infty^2 \| H \|_1 \varepsilon^L, \\
\text{Var}_\theta C &\leq \text{Var}_{R,L} \partial_\theta C + \frac{f(\varepsilon^L, \| H \|_1 \varepsilon^L)}{2^n},
\end{align*}
\]

where we use the shorthand $\varepsilon^L := \varepsilon^L_{U_R}$ and $\varepsilon^L := \varepsilon^L_{U_L}$ and with $f(x,y)$ defined in Eq. (17).

Again, Theorem 2 formally establishes that highly expressive ansätze experience flatter cost landscapes. Furthermore, a relation similar to (18) can be derived from Theorem 2. Hence, Theorem 2 also provides an extension of the barren plateau result of Ref. [27]. However, since $\| H \|_\infty^2 \in \mathcal{O}(1)$ for all $H$, (19) does not experience the same looseness for local costs of large systems as (14). On the other hand, since $\| H \|_1$ may scale exponentially in $n$, (20) may become loose for large systems and therefore we expect (15) to generally be more useful than (20).

**B. Numerical Simulations**

Since the analytic bounds in the previous section are upper bounds, we have no guarantee that inexpressive
ansätzte will exhibit larger cost gradients. The bounds thus leave open the question of whether/how reducing the expressibility of an ansatz changes the cost landscape. Moreover, they leave open the question of how one can avoid the barren plateau phenomenon that is observed for maximally expressive ansätzte.

One can conceive of numerous ways in which the expressibility of an ansatz can be tuned, each of which could have a different impact. In this section, we consider four such ways: decreasing the depth of the circuits, correlating circuit parameters, and restricting either the direction or angle of rotations. We then numerically investigate the effect these have on the cost gradient scaling.

For completeness, in our numerics we consider both a 2-local cost where the measurement operator is composed of Pauli-$z$ measurements on the first and second qubits, $H_L = \sigma_1^z \sigma_2^z$, and a global cost where the measurement operator consists of Pauli-$z$ measurements across all qubits, $H_G = \bigotimes_{i=1}^n \sigma_i^z$ [28]. In both cases, following [27], the system is prepared in the pure state, $\rho = |\psi_0\rangle \langle \psi_0| \otimes n$ where $|\psi_0\rangle = \exp(-i(\pi/8)\sigma_Y)|0\rangle$. We further consider a layered hardware efficient ansatz,

$$U(k_l, \theta_l, D) := \prod_{l=1}^{D} W V(k_l, \theta_l),$$

consisting of $D$ alternating layers of random single qubit gates and entangling layers as shown in Fig. 2. Specifically, the entangling layer,

$$W = \prod_{i=1}^{n-1} \text{C-Phase}_{i,i+1},$$

is composed of a ladder of controlled-phase operations, C-Phase, between adjacent qubits in a 1-dimensional array. The single-qubit layer consists of a series of random single qubit rotations

$$V(k_l, \theta_l) = \prod_{i=1}^{n} R_{k_i}^l(\theta_i^l),$$

where $R_{k_i}^l(\theta_i^l)$ is a rotation of the $i_{th}$ qubit by an angle $\theta_i^l$ about the $k_i$ axis. In the maximally expressive version of the ansatz the $x$, $y$, or $z$ rotation directions $\{k_i\}$ for each qubit on each layer are chosen independently and with equal probability, and the rotation angles $\{\theta_i^l\}$ are independently and randomly chosen in the range $0$ to $2\pi$.

The results presented here are extended in Appendix F, where we study the correlation between cost gradient and the expressibility measures $\varepsilon_R^l$ and $\varepsilon_L^l$. These results demonstrate a clear correlation between expressibility and cost gradients, with the Hamiltonian-dependent expressibility measure $\varepsilon_L^l$ capturing the dependence of cost gradients on the locality of the measurement operator $H$.

**Circuit depth.** One of the simplest ways of reducing the expressibility of an ansatz is reducing the depth $D$ of the circuit. It was shown in [28] that global costs with a hardware efficient ansatz experience barren plateaus irrespective of the depth of the circuit. However, local costs only exhibit barren plateaus for deep circuits ($D \in \Omega(\text{poly}(n))$) but are trainable for shallow circuits ($D \in \mathcal{O}(\log(n))$).

We obtain similar results here. As shown in Fig. 3(A), for the global cost the variance in the partial derivative is seemingly independent of the depth of the circuit and vanishes exponentially with the size of the system $n$. Conversely for local costs, as shown in Fig. 3(D), exponentially vanishing partial derivatives are observed for systems up to 12 qubits for depths $D \gtrapprox 100$. However shallow circuits $D \lesssim 50$ exhibit an approximately constant scaling for $n \gtrapprox 8$.

**Correlating parameters.** A more sophisticated means of reducing the expressibility of the ansatz is to correlate the rotation angles [37]. Here we consider three different means of correlating parameters, as sketched in Fig. 2, and plot the corresponding variance in the cost partial derivative in the central panel of Fig. 3. In the first, shown in yellow, we correlate the qubits (but allow the angles to vary between layers), i.e., $k_i = k_l^i$ and $\theta_i = \theta_l^i$ for any two qubits $i$ and $i'$. In the second (plotted in green) we correlate the different layers (but not the qubits), i.e., $k_i^l = k_l$ and $\theta_i^l = \theta_l^i$, for any two layers $l$ and $l'$. Finally, as shown in blue, we correlate both the qubits and layers. In this case all the qubits rotate in the same direction and by the same angle, i.e., $k_i^l = k_l^i$ and $\theta_i^l = \theta_l^i$ for any two qubits $i$ and $i'$ and layers $l$ and $l'$. In other words, all parameters are correlated. The data for only $y(x)$ rotations is indicated by the solid (dashed) lines respectively.

In contrast to varying circuit depth, here we obtain similar results irrespective of whether a local or global cost is used. Correlating both the qubits and the layers results in the least expressive ansatz and correspondingly the largest variation in cost gradients is observed. Indeed, in this case the variance in the cost gradient is approximately constant. In contrast, correlating just the qubits, or just the layers, increases the cost gradients and
Local Cost
Global Cost
\[ \partial \text{Var} \theta C \]

FIG. 3. Partial derivative scalings for different expressibilities. The variance in the partial derivative of a global cost with \( H_G = \bigotimes_{i=1}^n \sigma_i \) (top) and 2-local cost with \( H_L = \sigma_i \sigma_j \) (bottom) as a function of the number of qubits \( n \) (in both cases \( \rho = |\psi_0\rangle \langle \psi_0| \)) where \( |\psi_0\rangle = \exp(-i\pi/8\sigma_y)|0\rangle \)). In the left panel we vary the circuit depth \( D \) of a hardware efficient ansatz. In the right (middle) panel we consider the effect of correlating parameters (restricting the directions of rotation) of a hardware efficient ansatz with \( D = 150 \) with the choices of correlations (rotations) indicated in the figure legend. In all cases the derivative is taken with respect to \( \theta_1 \), the rotation angle of the first qubit in the first layer, and the variance is taken over an ensemble of 1000 unitaries.

Here we randomly initialize the parameters by randomly choosing \( \theta_i \) in the range \([0, 2\pi]\). We find the cost partial derivatives for different \( r \) values perfectly overlap in this case, i.e., for a random initialization, restricting the ansatz to a limited range of rotation angles does not change the partial derivatives observed.

On the other hand, if the parameters are initialized close to the solution, varying \( r \) has a substantial effect on the observed partial derivatives for local costs, and a reduced effect for global costs. This is seen in (B) and (C) of Fig. 4 where we initialize to identity, i.e., pick \( \theta_i = 0 \) for all \( i \), which is close to the solution for this simple problem. In this case, for \( r \) close to 1 (as shown in red and yellow) the variance in the partial derivative again vanishes exponentially with \( n \). However, for small angle ranges, \( r \lesssim 0.1 \), as shown in blue, we find that the partial derivative of a local cost ceases to exhibit an exponential scaling. To some degree, a similar effect is displayed for global costs; however, the effect is reduced and is only visible in the data here for \( r \approx 0.025 \).

This change in partial derivative scaling for small \( r \) for initializations close to the solution is plausibly explained by the fact that the global minimum of costs exhibiting barren plateaus tend to sit within a steep and narrow gorge [28], as sketched in Fig. 1(C). By initializing close to the solution we are likely to be initializing within the narrow gorge. In this case, when \( r \) is close to 1 the ansatz still explores the entire cost landscape and therefore the variance in the partial derivative will be unchanged. However, for smaller \( r \) the ansatz is constrained to the region around the the narrow gorge itself, and hence a larger variance in partial derivatives is observed.

Restricting rotation angles. A final way to reduce the expressibility of an ansatz is by reducing the range the rotation angles \( \theta \) are chosen from. That is, choosing the \( \theta_i \) in the range \([\tilde{\theta}_i, \tilde{\theta}_i + 2\pi r]\) where \( \tilde{\theta}_i \) is a fixed initialization point. For \( r = 1 \) the ansatz explores the entire solution space but for \( r < 1 \) the ansatz is constrained to exploring a subset of the solution space where the rotation angles \( \theta_i \) deviate from \( \tilde{\theta}_i \) by at most \( 2\pi r \).

However, with a little thought, it is clear that, in contrast to the previous three approaches we have discussed, restricting the rotation angles of the ansatz does not change the cost landscape but rather limits the region of the landscape explored by the ansatz. Thus, in general, reducing the rotation angles does not affect the cost gradients experienced. This intuition is confirmed by the numerical results displayed in the top panel of Fig. 4.
Partial derivative scalings for restricted angle ranges. The scaling of the variance in the partial derivative when the rotation angles $\theta_l$ are randomly chosen from the range $[0, \pi + 2\pi r]$, such that for $r = 1$ (red) the ansatz explores the entire solution space but for $r \ll 1$ (blue) the ansatz is constrained to exploring close to the initialization point defined by $\{ \tilde{\theta}_l \}$. In (A), the angles $\{ \tilde{\theta}_l \}$ are fixed (randomly chosen) initialization point away from the solution (here we consider a local cost but the data for a global cost is essentially unchanged). In (B) and (C), which correspond to global and local costs respectively, the angles $\tilde{\theta}_l = 0$ for all $l$ and $i$, which is close to the global minimum of the cost. In all cases the derivative is taken with respect to $\theta_l$, the rotation angle of the first qubit in the first layer and the variance is taken over an ensemble of 1000 unitaries.

Outlook for ansatz design. Figure 3 suggests that reducing the depth of a circuit and correlating parameters are the most effective strategies for amplifying the observed cost gradients. However, the optimal solution, of course, may not lie within a shallow or highly correlated ansatz. When deep and/or uncorrelated circuits are required, as is expected to be the case for many problems of interest, then a perturbative strategy may instead be effective. That is, one could start the variational algorithm using a shallow, highly correlated ansatz and as the cost is iteratively minimized gradually grow the ansatz [8, 15, 38] and decorrelate the parameters [37].

Restricting the angle range also appears to provide an effective strategy for increasing cost gradients, but for it to be practical it is necessary to initialize close to the solution. This, of course, requires either prior knowledge of an approximate solution to the problem at hand or an effective pre-training strategy to obtain such an approximate solution. The viability of either of these options warrants further investigation.

IV. Discussion

In this work, we extended the well-known barren plateau result. This result was restricted to ansätze that form 2-designs [27], while we extended it to arbitrary ansätze in our Theorems 1 and 2. In practice, this extension may prove to be quite useful, since many ansätze of interest are not exact 2-designs but rather are some approximate notion of this [59–62]. Our results can potentially provide useful bounds on the variance of the gradient in this realistic scenario of approximate 2-designs. The key to our extension was to consider the expressibility of the ansatz, which has recently been precisely defined in terms of the distance of the distribution obtained through the ansatz from being a 2-design. Hence, our extension linked two key properties of ansätze: their expressibility and their gradient magnitudes. Our bounds demonstrate that increasing the expressibility of an ansatz can result in smaller cost gradients. We believe that this connection is very interesting, and there is certainly much more to be explored along these lines. One natural question is whether our bounds can be further tightened.

To go beyond our bounds and look at the precise relation between expressibility and gradients, we performed extensive numerics. We considered several different strategies by which one can vary the expressibility. We typically observed a strong correlation (especially for local cost functions) between the expressibility and the variance of the gradient. We direct the reader to Appendix F for further numerics demonstrating this correlation.

We remark that the numerical results presented here are necessarily problem specific, since they depend both on the choice in cost function and ansatz. Further work is required to ascertain the extent to which the trends observed here are universally observed. In particular it would be valuable to investigate whether any analytic results can be obtained to support them.

Nevertheless, there are several interesting trends shown in our numerics that even suggest potential strategies of avoiding or mitigating barren plateaus. As discussed above, correlating parameters and restricting rotation angles (especially when initializing near the solution) are two strategies that significantly mitigated barren plateaus in our numerics. Further exploring these and other strategies will be an important direction for future research.
Acknowledgments

ZH and PJC were supported by the Los Alamos National Laboratory (LANL) ASC Beyond Moore’s Law project. KS was supported by the Laboratory Directed Research and Development (LDRD) program of LANL under project number 20190065DR. MC was initially supported by the LDRD program of LANL under project number 20180628ECR, and also supported by the Center for Nonlinear Studies at LANL. This work was also supported by the U.S. Department of Energy (DOE), Office of Science, Office of Advanced Scientific Computing Research, under the Accelerated Research in Quantum Computing (ARQC) program.

[1] Frank Arute, Kunal Arya, Ryan Babbush, Dave Bacon, Joseph C Bardin, Rami Barends, Rupak Biswas, Sergio Boixo, Fernando GSL Brandao, David A Buell, et al., “Quantum supremacy using a programmable superconducting processor,” Nature 574, 505–510 (2019).
[2] John Preskill, “Quantum Computing in the NISQ era and beyond,” Quantum 2, 79 (2018).
[3] A. Peruzzo, J. McClean, P. Shadbolt, M.-H. Yung, X.-Q. Zhou, P. J. Love, A. Aspuru-Guzik, and J. L. O’Brien, “A variational eigenvalue solver on a photonic quantum processor,” Nature Communications 5, 4213 (2014).
[4] Jarrod R McClean, Jonathan Romero, Ryan Babbush, and Alán Aspuru-Guzik, “The theory of variational hybrid quantum-classical algorithms,” New Journal of Physics 18, 023023 (2016).
[5] Edward Farhi, Jeffrey Goldstone, and Sam Gutmann, “A quantum approximate optimization algorithm,” arXiv preprint arXiv:1411.4028 (2014).
[6] J. Romero, J. P. Olson, and A. Aspuru-Guzik, “Quantum autoencoders for efficient compression of quantum data,” Quantum Science and Technology 2, 045001 (2017).
[7] Sumeet Khatri, Ryan LaRose, Alexander Poremba, Lukasz Cincio, Andrew T Sornborger, and Patrick J Coles, “Quantum-assisted quantum compiling,” Quantum 3, 140 (2019).
[8] R. LaRose, A. Tikku, É. O’Neel-Judy, L. Cincio, and P. J. Coles, “Variational quantum state diagonalization,” npj Quantum Information 5, 1–10 (2018).
[9] Andrew Arrasmith, Lukasz Cincio, Andrew T Sornborger, Wojciech H Zurek, and Patrick J Coles, “Variational consistent histories as a hybrid algorithm for quantum foundations,” Nature communications 10, 1–7 (2019).
[10] M. Cerezo, Alexander Poremba, Lukasz Cincio, and Patrick J Coles, “Variational quantum fidelity estimation,” Quantum 4, 248 (2020).
[11] Kunal Sharma, Sumeet Khatri, M. Cerezo, and Patrick J Coles, “Noise resilience of variational quantum compiling,” New Journal of Physics 22, 043006 (2020).
[12] Carlos Bravo-Prieto, Ryan LaRose, Marco Cerezo, Yigit Subasi, Lukasz Cincio, and Patrick Coles, “Variational quantum linear solver,” arXiv preprint arXiv:1909.05820 (2019).
[13] M Cerezo, Kunal Sharma, Andrew Arrasmith, and Patrick J Coles, “Variational quantum state eigensolver,” arXiv preprint arXiv:2004.01372 (2020).
[14] Kentaro Heya, Ken M Nakamishi, Kosuke Mitarai, and Keisuke Fujii, “Subspace variational quantum simulator,” arXiv preprint arXiv:1904.08566 (2019).
[15] Cristina Cirstoiu, Zoe Holmes, Joseph Iscove, Lukasz Cincio, Patrick J Coles, and Andrew Sornborger, “Variational fast forwarding for quantum simulation beyond the coherence time,” npj Quantum Information 6, 1–10 (2020).
[16] Benjamin Commeau, M. Cerezo, Zoë Holmes, Lukasz Cincio, Patrick J Coles, and Andrew Sornborger, “Variational hamiltonian diagonalization for dynamical quantum simulation,” arXiv preprint arXiv:2009.02559 (2020).
[17] Ying Li and Simon C Benjamin, “Efficient variational quantum simulator incorporating active error minimization,” Physical Review X 7, 021050 (2017).
[18] Suguru Endo, Jizhao Sun, Ying Li, Simon C Benjamin, and Xiao Yuan, “Variational quantum simulation of general processes,” Physical Review Letters 125, 010501 (2020).
[19] Xiao Yuan, Suguru Endo, Qi Zhao, Ying Li, and Simon C Benjamin, “Theory of variational quantum simulation,” Quantum 3, 191 (2019).
[20] M. Cerezo, Andrew Arrasmith, Ryan Babbush, Simon C Benjamin, Suguru Endo, Keisuke Fujii, Jarrod R McClean, Kosuke Mitarai, Xiao Yuan, Lukasz Cincio, and Patrick J Coles, “Variational quantum algorithms,” arXiv preprint arXiv:2012.09265 (2020).
[21] Stuart Hadfield, Zhihui Wang, Bryan O’Gorman, Eleanor G Rieffel, Davide Venturelli, and Rupak Biswas, “From the quantum approximate optimization algorithm to a quantum alternating operator ansatz,” Algorithms 12, 34 (2019).
[22] Rodney J Bartlett and Monika Musiał, “Coupled-cluster theory in quantum chemistry,” Reviews of Modern Physics 79, 291 (2007).
[23] Joonho Lee, William J Huggins, Martin Head-Gordon, and K Birgitta Whaley, “Generalized unitary coupled cluster wave functions for quantum computation,” Journal of chemical theory and computation 15, 311–324 (2018).
[24] Yudong Cao, Jonathan Romero, Jonathan P Olson, Matthias Degroote, Peter D Johnson, Mária Kieferová, Ian D Kivlichan, Tim Menke, Borja Peropadre, Nicolas PD Sawaya, et al., “Quantum chemistry in the age of quantum computing,” Chemical reviews 119, 10856–10915 (2019).
[25] Dave Wecker, Matthew B Hastings, and Matthias Troyer, “Progress towards practical quantum variational algorithms,” Physical Review A 92, 042303 (2015).
[26] A. Kandala, A. Mezzacapo, K. Temme, M. Takita, M. Brink, J. M. Chow, and J. M. Gambetta, “Hardware-efficient variational quantum eigensolver for small molecules and quantum magnets,” Nature 549, 242 (2017).
[27] Jarrod R McClean, Sergio Boixo, Vadim N Smelyanskiy, Ryan Babbush, and Hartmut Neven, “Barren plateaus in quantum neural network training landscapes,” Nature
Kishor Bharti and Tobias Haug, “Iterative quantum assisted eigensolver,” arXiv preprint arXiv:2010.05638 (2020).

Kishor Bharti and Tobias Haug, “Quantum assisted simulator,” arXiv preprint arXiv:2011.06911 (2020).

Sukin Sim, Peter D. Johnson, and Alán Aspuru-Guzik, “Expressibility and entangling capability of parameterized quantum circuits for hybrid quantum-classical algorithms,” Advanced Quantum Technologies 2, 1900070 (2019).

Kouhei Nakaji and Naoki Yamamoto, “Expressibility of the alternating layered ansatz for quantum computation,” arXiv preprint arXiv:2005.12537 (2020).

Jirawat Tangpapanitanon, Supanut Thanasilp, Ninnat Dangniam, Marc-Antoine Lemoine, and Dimitris G Angelakis, “Expressibility and trainability of parameterized analog quantum systems for machine learning applications,” arXiv preprint arXiv:2005.11222 (2020).

Jacob Biamonte, Peter Wittek, Nicola Pancotti, Patrick Rebentrost, Nathan Wiebe, and Seth Lloyd, “Quantum machine learning,” Nature 549, 195–202 (2017).

Maria Schuld, Ilya Sinayskiy, and Francesco Petruccione, “An introduction to quantum machine learning,” Contemporary Physics 56, 172–185 (2015).

Kyle Poland, Kerstin Beer, and Tobias J Osborne, “No free lunch for quantum machine learning,” arXiv preprint arXiv:2003.14103 (2020).

Kunal Sharma, M. Cerezo, Zoë Holmes, Lukasz Cincio, and Patrick J Coles, “Reformulation of the no-free-lunch theorem for entangled data sets,” arXiv preprint arXiv:2007.04900 (2020).

D. P. DiVincenzo, D. W. Leung, and B. M. Terhal, “Quantum data hiding,” IEEE Transactions on Information Theory 48, 580–598 (2002).

D. Gross, K. Audenaert, and J. Eisert, “Evenly distributed unitaries: On the structure of unitary designs,” Journal of Mathematical Physics 48, 052104 (2007).

Daniel A. Roberts and Beni Yoshida, “Chaos and complexity by design,” Journal of High Energy Physics 2017, 121 (2017).

Richard A. Low, Pseudo-randomness and Learning in Quantum Computation, Ph.D. thesis, - (2010).

Nicholas Hunter-Jones, “Unitary designs from statistical mechanics in random quantum circuits,” arXiv preprint arXiv:1905.12053 (2019).

Aram W. Harrow and Richard A. Low, “Random quantum circuits are approximate 2-designs,” Communications in Mathematical Physics 291, 257–302 (2009).

Winton Brown and Omar Fawzi, “Scrambling speed of random quantum circuits,” arXiv preprint arXiv:1210.6644 (2012).

Aram Harrow and Saeed Mehraban, “Approximate unitary t-designs by short random quantum circuits using nearest-neighbor and long-range gates,” arXiv preprint arXiv:1809.06957 (2018).

Fernando G. S. L. Brandão, Aram W. Harrow, and Michal Horodecki, “Local random quantum circuits are approximate polynomial-designs,” Communications in Mathematical Physics 346, 397–434 (2016).

Zbigniew Puchała and Jarosław Adam Miszczak, “Symmetric integration with respect to the haar measure on the unitary groups,” Bulletin of the Polish Academy of Sciences Technical Sciences 65, 21–27 (2017).
Appendices

We begin by reviewing some definitions and prior results relevant for the rest of the appendices. We then provide proofs for the main results and theorems.

A. Preliminaries

Operator Norms. Let $D(H)$ denote the set of density operators acting on a Hilbert space $H$, i.e., those that are positive semi-definite with unit trace. Let $L(H)$ denote the space of square linear operators acting on $H$. The trace norm or Schatten 1-norm $\|\Omega\|_1$ of an operator $\Omega \in L(H)$ is defined as $\|\Omega\|_1 := \text{Tr}[\|\Omega\|_2]$, where $\|\Omega\|_2 := \sqrt{\text{Tr}(\Omega^2)}$. More generally, the Schatten $p$-norm of an operator $\Omega$ can be defined as $\|\Omega\|_p = (\text{Tr}[\|\Omega\|_2^p])^{1/p}$, which satisfies $\|\Omega\|_p \leq \|\Omega\|_q$ for $p \geq q$. The diamond norm of a Hermiticity preserving linear map $S_A$ is defined as

$$\|S_A\|_\diamond = \sup_n \sup_{\Omega_{AB} \neq 0} \frac{\|(S_A \otimes I_B)(\Omega_{AB})\|_1}{\|\Omega_{AB}\|_1},$$

(A1)

where $\Omega_{AB} \in L(H_A \otimes H_B)$ and $I_B$ denote an identity channel acting on an $n$-dimensional system $B$. The diamond-norm distance $\|N - M\|_\diamond$ is a measure of the distinguishability of two quantum operations $N$ and $M$.

Properties of the Haar measure. Let $U(d)$ denote the unitary group of degree $d = 2^n$. Let $d\mu_H(V) = d\mu(V)$ be the volume element of the Haar measure, where $V \in U(d)$. The volume of the Haar measure is finite: $\int_{U(d)} d\mu(V) < \infty$. The Haar measure is uniquely defined up to a multiplicative constant factor. Let $d\zeta(V)$ be an invariant measure. Then there exists a constant $c$ such that $d\zeta(V) = c \cdot d\mu(V)$. The Haar measure is left- and right-invariant under the action of the unitary group of degree $d$, i.e., for any integrable function $g(V)$, the following holds:

$$\int_{U(d)} d\mu(V) g(WV) = \int_{U(d)} d\mu(V) g(VW) = \int_{U(d)} d\mu(V) g(V),$$

(A2)

where $W \in U(d)$.

Symbolic integration. We recall formulas which allow for the symbolical integration with respect to the Haar measure on a unitary group [63]. For any $V \in U(d)$ the following expressions are valid for the first two moments:

$$\int d\mu(V) v_{ij} v_{ik}^* = \frac{\delta_{ij}\delta_{jk}}{\sqrt{d}},$$

$$\int d\mu(V) v_{i1j1} v_{i2j2} v_{i1j1}^* v_{i2j2}^* = \frac{\delta_{i1i2}\delta_{j1j2} - \delta_{i1j2}\delta_{i2j1} + \delta_{i2j1}\delta_{i1j2} + \delta_{i1i2}\delta_{j1j2}}{d(d^2-1)},$$

(A3)

where $v_{ij}$ are the matrix elements of $V$. Assuming $d = 2^n$, we use the notation $i = (i_1, \ldots, i_n)$ to denote a bitstring of length $n$ such that $i_1, i_2, \ldots, i_n \in \{0, 1\}$.

Useful Identities. We use the following identities, which can be derived using Eq. (A3) (see [28] for a review):

$$\int d\mu(W) \text{Tr}[WAW^\dagger B] = \frac{\text{Tr}[A] \text{Tr}[B]}{d},$$

(A4)

$$\int d\mu(W) \text{Tr}[WAW^\dagger BWCW^\dagger D] = \frac{\text{Tr}[A] \text{Tr}[C] \text{Tr}[BD] + \text{Tr}[AC] \text{Tr}[B] \text{Tr}[D]}{d^2-1} - \frac{\text{Tr}[AC] \text{Tr}[BD] + \text{Tr}[A] \text{Tr}[B] \text{Tr}[C] \text{Tr}[D]}{d(d^2-1)},$$

(A5)

$$\int d\mu(W) \text{Tr}[WAW^\dagger B] \text{Tr}[WCW^\dagger D] = \frac{\text{Tr}[A] \text{Tr}[B] \text{Tr}[C] \text{Tr}[D] + \text{Tr}[AC] + \text{Tr}[BD]}{d^2-1} - \frac{\text{Tr}[AC] \text{Tr}[B] \text{Tr}[D] + \text{Tr}[A] \text{Tr}[C] \text{Tr}[BD]}{d(d^2-1)},$$

(A6)

where $A, B, C,$ and $D$ are linear operators on a $d$-dimensional Hilbert space.

Let $A \in L(H)$ and $B \in L(H')$. Then the following identity holds:

$$\text{Tr}[A] \text{Tr}[B] = \text{Tr}[A \otimes B].$$

(A7)

Let $A, B \in L(H)$, where $H$ is a $d^2$-dimensional Hilbert space. Then from Eq. (A3), we derive the following integral:

$$\int d\mu(U) \text{Tr}[AU^\otimes 2 B U^\otimes 2] = \frac{\text{Tr}[A] \text{Tr}[B] + \text{Tr}[AW] \text{Tr}[BW]}{d^2-1} - \frac{\text{Tr}[AW] \text{Tr}[B] + \text{Tr}[A] \text{Tr}[BW]}{d(d^2-1)},$$

(A8)

where $W$ is the subsystem swap operator, i.e., $W|i⟩|j⟩ = |j⟩|i⟩$. 


B. Definitions of Expressibility

In broad terms a parameterized quantum circuit can be considered expressive if the circuit can be used to uniformly explore the unitary group \( \mathcal{U}(d) \). Thus, the expressibility of a circuit can be defined in terms of the following superoperator

\[
\mathcal{A}_U^{(t)}(\cdot) := \int_{\mathcal{U}(d)} d\mu(V) V^{\otimes t}(\cdot)(V^{\dagger})^{\otimes t} - \int_{\mathcal{U}} dU U^{\otimes t}(\cdot)(U^{\dagger})^{\otimes t}
\]  

(B1)

where \( d\mu(V) \) is the volume element of the Haar measure and \( dU \) is the volume element corresponding to the uniform distribution over \( \mathcal{U} \). If \( \mathcal{A}_U^{(t)}(X) = 0 \) for all operators \( X \) then the averaging over elements of \( \mathcal{U} \) agrees with averaging over the Haar distribution up to the \( t \)-th moment. In this case \( \mathcal{U} \) is said to form a \( t \)-design. For our purposes it suffices to consider the behavior of \( \mathcal{A}_U^{(t)} \) for \( t = 2 \). Henceforth, we drop the \( t \)-superscript and denote \( \mathcal{A}_U^{(2)}(\cdot) \) as \( \mathcal{A}_U(\cdot) \). In the context of minimizing a generic cost \( C \) of the form specified by Eq. (1), we are interested in the quantities

\[
\varepsilon_U^\rho := ||\mathcal{A}_U(\rho^{\otimes 2})||_2 \quad \varepsilon_U^H := ||\mathcal{A}_U(H^{\otimes 2})||_2
\]  

(B2)

(B3)

The quantities \( \varepsilon_U^\rho \) and \( \varepsilon_U^H \) may be more readily computed by relating them to a generalization of the frame potential. To demonstrate how, let us first recall that the frame potential \([48, 56]\) of an ensemble \( \mathcal{U} \) may be more readily computed by relating them to a generalization of the frame potential. Thus, the expressiblity of a circuit can be defined in terms of the following super-

\[
\mathcal{F}_U := \int_{\mathcal{U}} \int_{\mathcal{U}} dU dV |\langle 0|UV^{\dagger}|0 \rangle|^4,
\]  

(B4)

where \( dU \) and \( dV \) are volume elements corresponding to the distribution over \( \mathcal{U} \). We then note that the quantity \( ||\mathcal{A}_U(|0\rangle\langle 0|)||_2^2 \) can be rewritten in terms of \( \mathcal{F}_U \) as follows

\[
||\mathcal{A}_U(|0\rangle\langle 0|)||_2^2 = \left\| \int_{\mathcal{U}(d)} d\mu(V) V^{\otimes 2}(0)\langle 0|V^{\dagger})^{\otimes 2} - \int_{\mathcal{U}} dU U^{\otimes 2}(0)\langle 0|U^{\dagger})^{\otimes 2} \right\|_2^2
\]  

(B5)

where we use the left and right invariance of the Haar measure, and where we defined

\[
\mathcal{F}_{\text{Haar}} := \int_{\mathcal{U}(d)} \int_{\mathcal{U}(d)} d\mu(U)d\mu(V)|\langle 0|UV^{\dagger}|0 \rangle|^4 = \frac{1}{(2^n + 1)2^{n-1}}
\]  

(B6)

In the context of the expressibility of a VQA we are interested in the more general quantity \( ||\mathcal{A}_U(X^{\otimes 2})||_2 \) where \( X \) is a quantum state \( \rho \) or Hamiltonian \( H \). Following the same approach as in Eq. (B5), we note that \( ||\mathcal{A}_U(X^{\otimes 2})||_2 \) can be rewritten as

\[
||\mathcal{A}_U(X^{\otimes 2})||_2 = \sqrt{\mathcal{F}_U(X) - \mathcal{F}_{\text{Haar}}(X)},
\]  

(B7)

where we have defined the operator dependent frame-potential as

\[
\mathcal{F}_U^{(X)} := \int_{\mathcal{U}} \int_{\mathcal{U}} d\mu(U)d\mu(V)|\langle 0|UV^{\dagger}|0 \rangle|^4
\]  

(B8)

and

\[
\mathcal{F}_{\text{Haar}}^{(X)} := \int_{\mathcal{U}(d)} \int_{\mathcal{U}(d)} d\mu(U)d\mu(V)|\langle 0|UV^{\dagger}|0 \rangle|^4.
\]  

(B9)

The latter can be evaluated using Eq. (A6) to give

\[
\mathcal{F}_{\text{Haar}}^{(X)} = \frac{\text{Tr}[X]^4 + \text{Tr}[X^2]^2 - 2\text{Tr}[X^2]\text{Tr}[X]^2}{2^{2n-1} - 1}.
\]  

(B10)
Thus our expressibility measures can be related to state and Hamiltonian dependent frame potentials via

\[ \varepsilon^\rho_U := \| A_U(\rho^\otimes 2) \|_2 = \sqrt{\mathcal{F}_U(\rho) - \mathcal{F}_U(\rho)_{\text{Haar}}} \]  

\[ \varepsilon^H_U := \| A_{U,H} \|_2 = \sqrt{\mathcal{F}_U(H) - \mathcal{F}_U(H)_{\text{Haar}}} \]  

We will use these expressions to evaluate the expressibility of different ansätze in Appendix F.

**C. Proof for Eq. (8)**

For a random layered parametrized ansatz of the form Eq. (2) and Eqs. (11)–(12), and the generic cost defined in Eq. (1), we now show that \( \langle \partial_k C \rangle_U = 0 \) for all \( k \) and therefore the cost landscape is unbiased.

To do so, let us first introduce the shorthand

\[ \tilde{\rho} = W_k \left( \prod_{j=1}^{k-1} U_j(\theta_j)W_j \right) \rho \left( \prod_{j=1}^{k-1} U_j(\theta_j)W_j \right)^\dagger \]  

\[ \tilde{H} = U_L(\theta)^\dagger H U_L(\theta). \]  

Then the cost function can be expressed as

\[ C = \text{Tr}[U_k(\theta_k)\tilde{\rho}U_k(\theta_k)^\dagger \tilde{H}], \]  

which implies that

\[ \partial_k C = -i \text{Tr}[V_k U_k(\theta_k)\tilde{\rho}U_k(\theta_k)^\dagger \tilde{H}] + i \text{Tr}[U_k(\theta_k)\tilde{\rho}U_k(\theta_k)^\dagger V_k \tilde{H}] \]  

\[ = -i \text{Tr}[V_k(\cos(\theta_k) - i \sin(\theta_k)V_k)\tilde{\rho}(\cos(\theta_k) + i \sin(\theta_k)V_k)] + i \text{Tr}[(\cos(\theta_k) - i \sin(\theta_k)V_k)\tilde{\rho}(\cos(\theta_k) + i \sin(\theta_k)V_k)V_k \tilde{H}] \]  

\[ = -i(\cos(\theta_k)^2 - \sin(\theta_k)^2)(\text{Tr}[V_k \tilde{\rho} \tilde{H}] + \text{Tr}[\tilde{\rho} V_k \tilde{H}]) \]  

Therefore, uniform averaging of \( \partial_k C \) over \( \theta_k \) leads to

\[ \frac{1}{2\pi} \int_0^{2\pi} d\theta_k \partial_k C = -\frac{i}{2\pi} \int_0^{2\pi} d\theta_k (\cos(\theta_k)^2 - \sin(\theta_k)^2)(\text{Tr}[V_k \tilde{\rho} \tilde{H}] + \text{Tr}[\tilde{\rho} V_k \tilde{H}]) \]  

\[ = 0 , \]  

which implies that \( \langle \partial_k C \rangle_U = 0 \).

**D. Variance of the partial derivative derivation**

For a random layered parametrized ansatz of the form Eqs. (2) and (11)–(12), and the generic cost defined in Eq. (1), the partial derivative of the cost can be written as

\[ \partial_k C := \frac{\partial C}{\partial \theta_k} = i \text{Tr}[U_R \tilde{\rho} U_R^\dagger [V_k, U_L^\dagger H U_L]] , \]  

where \( U_L \) and \( U_R \) are defined in Eq. (12).

Since the average derivative of the cost vanishes, as discussed in Appendix C, its variance is given by

\[ \text{Var} \partial_k C = \langle (\partial_k C)^2 \rangle_U . \]  

Eq. (D1) and Eq. (D2) provide the starting point to derive the bounds Eqs. (14)–(16) and Eqs. (19)–(21).
1. Bound in Eq. (14).

Note that two different ensembles $U_L$ and $U_R$ can be generated using $U_L(\theta)$ and $U_R(\theta)$, respectively, as defined in Eq. (11). Let $dU_L$ and $dU_R$ denote volume elements corresponding distributions over $U_L$ and $U_R$, respectively. Since $U_L$ and $U_R$ are independent, from the definition of $dU$ and from Eq. (11), we get that $dU = dU_LdU_R$.

Then by substituting Eq. (D1) into Eq. (D2) and using Eq. (A7), we get

$$
\text{Var}\partial_k C = -\int_{U_L} dU_L \int_{U_R} dU_R \text{Tr}[U_R^\otimes 2 \rho \otimes 2 U_R^\dagger \otimes 2 X_{Lk}^\otimes 2]
$$

where

$$X_{Lk} := [V_k, U_L^\dagger H U_L].$$

Next we substitute in $A_R(\rho \otimes 2)$ to give

$$\text{Var}\partial_k C = -\int_{U_L} dU_L \int_{U(d)} d\mu(U) \text{Tr}[U_R^\otimes 2 \rho \otimes 2 U_R^\dagger \otimes 2 X_{Lk}^\otimes 2] + \int_{U_L} dU_L \text{Tr}[A_R(\rho \otimes 2) X_{Lk}^\otimes 2]
$$

$$= \text{Var}_R \partial_k C + \int_{U_L} dU_L \text{Tr}[A_R(\rho \otimes 2) X_{Lk}^\otimes 2].
$$

Rearranging we are left with

$$|\text{Var} \partial_k C - \text{Var}_R \partial_k C| \leq \left| \int_{U_L} dU_L \text{Tr}[A_R(\rho \otimes 2) X_{Lk}^\otimes 2] \right|
$$

which on using the triangle inequality followed by the Cauchy-Schwarz inequality reduces to

$$|\text{Var} \partial_k C - \text{Var}_R \partial_k C| \leq \int_{U_L} dU_L |\text{Tr}[A_R(\rho \otimes 2) X_{Lk}^\otimes 2]|
$$

$$\leq \int_{U_L} dU_L ||X_{Lk}^\otimes 2||_2 ||A_R(\rho \otimes 2)||_2.
$$

The term $||X_{Lk}^\otimes 2||_2$ can be bounded as follows. First we note that $X_{Lk}^\dagger = -X_{Lk}$, which implies that

$$||X_{Lk}^\otimes 2||_2 = \sqrt{\text{Tr}[X_{Lk}^\otimes 2 X_{Lk}^\otimes 2]} = \sqrt{\text{Tr}[X_{Lk}^\dagger \otimes X_{Lk}^\otimes 2]} = |\text{Tr}[X_{Lk}^2]| = |\text{Tr}[[V_k, U_L^\dagger H U_L]|2]].
$$

Let $A = V_k$ and $B = U_L^\dagger H U_L$. Since $A$ and $B$ are Hermitian, from the triangle inequality and the Cauchy-Schwarz inequality, we get

$$|\text{Tr}[[A, B]^2]| = 2|\text{Tr}[ABAB] - \text{Tr}[A^2 B^2]| \leq 2(|\text{Tr}[ABAB]| + |\text{Tr}[B^2]|) \leq 2\sqrt{\text{Tr}([ABAABA][B^2]^2 + 2|\text{Tr}[B^2]| = 4|\text{Tr}[B^2]|}.
$$

Therefore, we find that

$$||X_{Lk}^\otimes 2||_2 \leq 4\text{Tr}([U_L^\dagger H U_L]^2]) = 4\text{Tr}[H^2] = 4||H||_2^2.
$$

Hence the bound takes the form

$$|\text{Var} \partial_k C - \text{Var}_R \partial_k C| \leq 4 \int_{U_L} dU_L ||A_R(\rho \otimes 2)||_2 ||H||_2^2 = 4||A_R(\rho \otimes 2)||_2 ||H||_2^2,
$$

which completes the proof.

Extension to generalized cost. This result can be further extended to cost functions of the following form

$$C(\theta) = \sum_m \text{Tr}[H_m U(\theta) \rho_m U(\theta)^\dagger],
$$

for which the derivative with respect to the parameter $\theta_k$ can be written as

$$\partial_k C = i \sum_m \text{Tr}[U_R^\dagger \rho_m U_R^\dagger [V_k, U_L^\dagger H_m U_L]].
$$
Therefore, from Eq. (D3) it follows that
\[
\text{Var} \partial_k C = - \sum_{m,n}^{U_L} \int dU_L \int_{U_R} dU_R \text{Tr}[U_R \otimes \rho_m (U_R^\dagger)^\otimes 2 \mathcal{X}^m_{Lk} \otimes \mathcal{X}^n_{Lk}],
\]
(D14)
where \( \mathcal{X}^m_{Lk} \) is defined in Eq. (D4) with \( H = H_m \).

After substituting \( \mathcal{A}_R(\rho_j \otimes \rho_k) \), we get
\[
\text{Var} \partial_k C = \text{Var}_R \partial_k C + \sum_{m,n}^{U_L} \int dU_L \text{Tr}[\mathcal{A}_R(\rho_m \otimes \rho_n)(\mathcal{X}^m_{Lk} \otimes \mathcal{X}^n_{Lk})],
\]
(D15)
which implies that
\[
|\text{Var} \partial_k C - \text{Var}_R \partial_k C| \leq \sum_{m,n}^{U_L} \int dU_L \text{Tr}[\mathcal{A}_R(\rho_m \otimes \rho_n)\mathcal{X}^m_{Lk} \otimes \mathcal{X}^n_{Lk}]| \leq \sum_{m,n}^{U_L} \int dU_L \|\mathcal{A}_R(\rho_m \otimes \rho_n)\| \|\mathcal{X}^m_{Lk} \otimes \mathcal{X}^n_{Lk}\|_2 \quad \text{(D16)}
\]
\[
\leq \sum_{m,n}^{U_L} \|\mathcal{A}_R(\rho_m \otimes \rho_n)\|_2 \sqrt{\text{Tr}[\mathcal{X}^m_{Lk} \otimes \mathcal{X}^n_{Lk}]} \quad \text{(D17)}
\]
\[
\leq 4 \sum_{m,n}^{U_L} \|\mathcal{A}_R(\rho_m \otimes \rho_n)\|_2 \|H_m\|_2 \|H_n\|_2 \quad \text{(D18)}
\]
where we used steps similar to those used in deriving Eqs. (D8)–(D11).

2. Bound in Eq. (15).

Substituting Eq. (D1) into Eq. (D2), using Eq. (A7), and the cyclicity of the trace operation, we find that
\[
\text{Var} \partial_k C = \int_{U_L} dU_L \int_{U_R} dU_R \text{Tr}[U_L^\otimes 2 H \otimes 2 U_L \otimes 2 Y_{Rk}^\otimes 2]
\]
(D20)
where \( Y_{Rk} := [U_R \rho U_R^\dagger, V_k] \). The rest of the derivation proceeds in the same manner as for the bound in Eq. (14).

Extension to generalized cost. Similar to Eq. (D19), the bound in Eq. (15) can be extended for the cost functions of the form in Eq. (D12). In particular, we find that
\[
|\text{Var} \partial_k C - \text{Var}_L \partial_k C| \leq 4 \sum_{m,n} \|\mathcal{A}_L(H_m \otimes H_n)\|_2 \|\rho_m\|_2 \|\rho_n\|_2 .
\]
(D21)

3. Bound in Eq. (16).

To derive Eq. (16) we start by substituting Eq. (D1) into Eq. (D2), using Eq. (A7), and the cyclicity of the trace operation to find that
\[
\text{Var} \partial_k C = - \int_{U_L} dU_L \int_{U_R} dU_R \text{Tr}[\mathcal{A}_R(\rho_R \otimes \rho_R^2) (V_k^\otimes 2 H_k^\otimes 2 + H_k^\otimes 2 V_k^\otimes 2 - 2(V_k \otimes 1) H_k^\otimes 2 (1 \otimes V_k))] \quad \text{(D22)}
\]
where we have introduced the short hand \( \rho_R := U_R \rho U_R^\dagger \) and \( H_L := U_L^\dagger H U_L \). Next we substitute in \( \mathcal{A}_L(H^\otimes 2) \) and \( \mathcal{A}_R(\rho^\otimes 2) \) to find that the variance is given by
\[
\text{Var} \partial_k C = \text{Var}_{L,R} \partial_k C - \text{Tr}[\mathcal{A}_R(\rho^\otimes 2) Z_{Lk}] + I_1 + I_2 .
\]
(D23)

Here we defined
\[
Z_{sk} := (V_k^\otimes 2 A_x(\omega_x) + A_x(\omega_x) V_k^\otimes 2 - 2(V_k \otimes 1) A_x(\omega_x)(1 \otimes V_k))
\]
(D24)
for $x = L$ and $x = R$, and where $\omega_R = \rho$ and $\omega_L = H$. The integrals $I_1$ and $I_2$ are given by

$$I_1 = \int_{\mathcal{U}(d)} d\mu(U) \text{Tr}[Z_{Lk} \tilde{\rho}^{\otimes 2}]$$
$$I_2 = \int_{\mathcal{U}(d)} d\mu(U) \text{Tr}[A_R(\rho^{\otimes 2})(V_k^{\otimes 2}) \hat{H}^{\otimes 2} + \hat{H}^{\otimes 2} V_k^{\otimes 2} - 2(V_k \otimes 1) \hat{H}^{\otimes 2}(1 \otimes V_k)].$$

(D25)

with $\tilde{\rho} = U \rho U^\dagger$ and $\tilde{H} = U^\dagger H U$.

The integrals $I_1$ and $I_2$ can be evaluated using Eq. (A8) as follows:

$$I_1 = \frac{1}{d^2 - 1} \text{Tr}[Z_{Lk} W] \text{Tr}[\rho^2] - \frac{1}{d(d^2 - 1)} \text{Tr}[Z_{Lk} W],$$
$$I_2 = \frac{1}{d^2 - 1} \text{Tr}[Z_{Rk} W] \text{Tr}[H^2] - \frac{1}{d(d^2 - 1)} \text{Tr}[Z_{Rk} W] \text{Tr}[H^2],$$

(D26)

where we used the fact that $\text{Tr}[Z_{Lk}] = \text{Tr}[Z_{Rk}] = 0$, $\text{Tr}[\rho^{\otimes 2} W] = \text{Tr}[\rho^2]$, and $\text{Tr}[H^{\otimes 2} W] = \text{Tr}[H^2]$.

Substituting these integrals, Eq. (D26), back into Eq. (D23) and then using the triangle inequality gives

$$|\text{Var}_{\partial C} - \text{Var}_{R, L, \partial \omega_C}| \leq \frac{1}{d^2 - 1} ((\text{Tr}[\rho^2] - 1/d) \text{Tr}[Z_{Lk} W] + (\text{Tr}[H^2] - \text{Tr}[H^2/d]) \text{Tr}[Z_{Rk} W]) + |\text{Tr}[A_R(\rho^{\otimes 2}) Z_{Lk}]|. \quad (D27)$$

Using Cauchy-Schwarz this reduces to

$$|\text{Var}_{\partial C} - \text{Var}_{R, L, \partial \omega_C}| \leq \frac{d}{d^2 - 1} \left( |\text{Tr}[\rho^2]|^2 - 1/d \right) ||Z_{Lk}||_2 + (||H||^2 - \text{Tr}[H^2/d] ||Z_{Rk}||_2) + ||A_R(\rho^{\otimes 2})||_2 ||Z_{Lk}||_2. \quad (D28)$$

where we have used $||W||_2 = d$. Finally, by expanding $||Z_{Lk}||_2$, using the triangle inequality and the fact that $V_k^2 = 1$ we find that

$$||Z_{Lk}||_2 \leq 4 \||A_R(\omega_x)||_2 \quad (D29)$$

for $x = L$ and $x = R$, and where $\omega_R = \rho$ and $\omega_L = H$. Thus we are left with

$$|\text{Var}_{\partial C} - \text{Var}_{R, L, \partial \omega_C}| \leq 4 ||A_R(\rho^{\otimes 2})||_2 ||A_L(H^{\otimes 2})||_2 + \frac{2^{n+2}}{2^m - 1} \left( ||A_R(\rho^{\otimes 2})||_2 (||H||_2^2 - \frac{1}{d} \text{Tr}[H^2]) + ||A_L(H^{\otimes 2})||_2 (||\rho||_2^2 - \frac{1}{d}) \right). \quad (D30)$$

**Extension to generalized cost.** Similar to Eqs. (D19) and (D21), the bound in Eq. (16) can be extended for the cost functions of the form in Eq. (D12). In particular, we find that

$$|\text{Var}_{\partial C} - \text{Var}_{R, L, \partial \omega_C}| \leq 4 \sum_{m, n} ||A_R(\rho_m \otimes \rho_n)||_2 ||A_L(H_m \otimes H_n)||_2$$
$$+ \frac{2^{n+2}}{2^m - 1} \sum_{m, n} \left( ||A_R(\rho_m \otimes \rho_n)||_2 \left( \text{Tr}[H_m H_n] - \frac{1}{d} \text{Tr}[H_m \text{Tr}[H_n]] \right) + ||A_L(H_m \otimes H_n)||_2 \left( \text{Tr}[\rho_m \rho_n] - \frac{1}{d} \right) \right). \quad (D31)$$

4. Reformulating bounds using the diamond norm.

Here we derive bounds Eqs. (19)-(21), in which the expressibility is quantified in terms of the diamond norm. This is a natural alternative way of formulating the bounds, since the diamond norm is an operationally meaningful measure of the distinguishability of two quantum operations that is often used to define $\epsilon$-approximate $t$-designs.

To derive Eq. (19) we start with Eq. (D7) and invoke the Holder’s inequality as follows:

$$|\text{Var}_{\partial C} - \text{Var}_{R, \partial \omega_C}| \leq \int_{\mathcal{U}_L} dU_L |\text{Tr}[A_R(\rho^{\otimes 2}) X_{Lk}^{\otimes 2}]|$$
$$\leq \int_{\mathcal{U}_L} dU_L ||X_{Lk}^{\otimes 2}||_\infty ||A_R(\rho^{\otimes 2})||_1. \quad (D32)$$
The term \( |X_L^{\otimes 2}|_\infty \) can now be bounded as follows. Given that \( X_L^1 = -X_L \), it follows from the unitary invariance and sub-multiplicativity of the infinity norm that
\[
|X_L^{\otimes 2}|_\infty = (|X_L|_\infty)^2 \leq (2|V_k|_\infty|U_L^H U_L|_\infty)^2 = (2|V_k|_\infty|H|_\infty)^2 \leq 4|H|_\infty^2.
\]
We additionally note that \( |\mathcal{E}(X)|_1 \leq |X|_1 |\mathcal{E}|_1 \) for any channel \( \mathcal{E} \) and operator \( X \), therefore
\[
|\mathcal{A}_R(\rho^{\otimes 2})|_1 \leq \|\rho\|_1 |\mathcal{A}_{U_R}|_\infty = |\mathcal{A}_{U_R}|_\infty := \varepsilon_R.
\]
Thus we are now left with
\[
|\text{Var}_R \partial_k C - \text{Var}_R \partial_k C| \leq 4|H|_\infty^2 \varepsilon_R.
\]
The derivation of Eq. (20) is entirely analogous.

To derive Eq. (21) we start with Eq. (D27) and again use Holder’s inequality in terms of the infinity and one norm to find
\[
|\text{Var}_R \partial_k C - \text{Var}_R \partial_k C| \leq \frac{1}{d^2 - 1}((|\rho|_2^2 - 1/d)|Z_{Lk}|_1 + (|H|_2^2 - \text{Tr}[H]^2/d)|Z_{Rk}|_1) + |\mathcal{A}_R(\rho^{\otimes 2})|_1 |Z_{Lk}|_\infty,
\]
where we have used \( |W|_\infty = 1 \). Finally, by expanding \( |Z_{xk}|_\infty \), using the triangle inequality and the fact that \( V_k^2 = 1 \) we find that
\[
|Z_{xk}|_\infty \leq |V_k^{\otimes 2} A_x(\omega_x)|_\infty + |A_x(\omega_x) V_k^{\otimes 2}|_\infty + 2(|V_k \otimes 1) A_x(\omega_x) (1 \otimes V_k)|_\infty
\leq 2|V_k^{\otimes 2}|_\infty|A_x(\omega_x)|_\infty + 2(|V_k \otimes 1)|_\infty|A_x(\omega_x)|_\infty(|1 \otimes V_k)|_\infty
\leq 4|A_x(\omega_x)|_\infty
\]
for \( x = L \) and \( x = R \). We additionally note that \( |\mathcal{E}(X)|_1 \leq |X|_1 |\mathcal{E}|_1 \) for any channel \( \mathcal{E} \) and operator \( X \), therefore,
\[
|\mathcal{A}_R(\rho^{\otimes 2})|_1 \leq |\mathcal{A}_R(\rho^{\otimes 2})|_1 \leq \varepsilon_R.
\]
Thus we are left with
\[
|\text{Var}_R \partial_k C - \text{Var}_R \partial_k C| \leq \frac{4}{d^2 - 1}((|\rho|_2^2 - 1/d)|\mathcal{A}_L(H)|_\infty + (|H|_2^2 - \text{Tr}[H]^2/d)|\mathcal{A}_R(\rho^{\otimes 2})|_1 + 4|\mathcal{A}_R(\rho)|_1 |\mathcal{A}_L(\rho^{\otimes 2})|_\infty
\]
or alternatively
\[
|\text{Var}_R \partial_k C - \text{Var}_R \partial_k C| \leq \frac{4}{d^2 - 1}((|\rho|_2^2 - 1/d)|H|_1 \varepsilon_L^2 + (|H|_2^2 - \text{Tr}[H]^2/d)\varepsilon_L^2) + 4|H|_1 \varepsilon_R^2 \varepsilon_L^2.
\]

### E. Variance in partial derivative for exact 2-designs.

In this Appendix, we provide the explicit expressions and the derivation of the variance in the partial derivative for a random layered parametrized ansatz of the form Eqs. (2) and (11)–(12), and the generic cost defined in Eq. (1). These quantities have been investigated in [27]; however, only the highest order terms in \( n \) were given. Here we provide higher order terms for completeness.

**Explicit expressions** Let us denote the variance of the cost when just \( U_R \), just \( U_L \), and both \( U_R \) and \( U_L \) form 2-designs as \( \text{Var}_R \partial_k C \), \( \text{Var}_L \partial_k C \), and \( \text{Var}_{R,L} \partial_k C \), respectively. These variances are given by
\[
\text{Var}_x \partial_k C = \frac{g_x(\rho, H, U)}{2^n - 1},
\]
where
\[
g_R(\rho, H, U) = -\left( \text{Tr}(\rho^2) - \frac{1}{2^n} \right) \int dU_L \text{Tr}([V_k, U_L^H U_L]^2)
\]
\[
g_L(\rho, H, U) = -\left( \text{Tr}(H^2) - \frac{1}{2^n} \text{Tr}[H]^2 \right) \int dU_R \text{Tr}([V_k, U_R^H U_R]^2)
\]
\[
g_{R,L}(\rho, H, U) = -2 \left( \text{Tr}(\rho^2) - \frac{1}{2^n} \right) \left( \frac{1}{2^n - 1} \text{Tr}(V_k^2) \text{Tr}(H^2) + \text{Tr}(V_k^2) \text{Tr}(H)^2 \right)
\]-
\[
- \frac{1}{2^n (2^n - 1)} \left[ \text{Tr}(V_k^2) \text{Tr}(H^2) + \text{Tr}(V_k^2) \text{Tr}(H)^2 \right] - \frac{1}{2^n} \text{Tr}(V_k^2) \text{Tr}(H^2)
\]

From Eq. (D1), we have
\[
\partial_k C := \frac{\partial C}{\partial \theta_k} = i \text{Tr}[U_R \rho U_R^\dagger [V_k, U_L^\dagger H U_L]].
\] (E5)

Since the cost gradient is unbiased, as in Eq. (8), the variance in the partial derivative is given by
\[
\text{Var}_k C = -\int dU_L \int dU_R \text{Tr}(U_R \rho U_R^\dagger [V_k, U_L^\dagger H U_L])^2.
\] (E6)

Then \(\text{Var}_R \partial_k C, \text{Var}_L \partial_k C,\) and \(\text{Var}_{R,L} \partial_k C\) can be calculated by the integration in Eq. (E6) over \(U_R, U_L,\) and both \(U_R\) and \(U_L,\) respectively.

Integrating over only \(U_R\) gives
\[
\text{Var}_R \partial_k C = -\frac{1}{d^2 - 1} \int dU_L \langle \text{Tr}(\rho^2 \text{Tr}([V_k, U_L^\dagger H U_L])^2 + \text{Tr}(\rho^2 \text{Tr}([V_k, U_L^\dagger H U_L]^2)) + \frac{1}{d(d^2 - 1)} \int dU_L \text{Tr}([V_k, U_L^\dagger H U_L]^2) \rangle
\] (E7)

\[
= -\frac{1}{d^2 - 1} \int dU_L \text{Tr}(\rho^2 \text{Tr}([V_k, U_L^\dagger H U_L]^2)) + \frac{1}{d(d^2 - 1)} \int dU_L \text{Tr}([V_k, U_L^\dagger H U_L]^2)
\] (E8)

\[
= -\left(\text{Tr}(\rho^2) - \frac{1}{d}\right) \left(\frac{1}{d^2 - 1}\right) \int dU_L \text{Tr}([V_k, U_L^\dagger H U_L]^2),
\] (E9)

where the first equality follows from Eq. (A6) and the second equality follows from the fact that the trace of a commutator is always zero.

Form the cyclicity of the trace operation and the arguments similar to Eqs. (E7) and (E8), we get
\[
\text{Var}_L \partial_k C = -\left(\text{Tr}(H^2) - \frac{\text{Tr}[H]^2}{d}\right) \left(\frac{1}{d^2 - 1}\right) \int dU_R \text{Tr}([V_k, U_R^\dagger H U_R]^2).
\] (E10)

In order to calculate \(\text{Var}_{R,L} \partial_k C,\) we note that \(\text{Tr}([V_k, U_L^\dagger H U_L]^2)\) in Eq. (E9) can be written as
\[
\text{Tr}([V_k, U_L^\dagger H U_L]^2) = 2\text{Tr}(U_L V_k U_L^\dagger H U_L V_k U_L^\dagger H) - \text{Tr}(U_L V_k^2 U_L^\dagger H^2).
\] (E11)

The integral of the first term over \(U_L\) in Eq. (E11) can be calculated using Eq. (A5) as follows:
\[
\int dU_L \text{Tr}(U_L V_k U_L^\dagger H U_L V_k U_L^\dagger H)
\]
\[
= \frac{1}{d^2 - 1} \left[\text{Tr}(V_k^2) \text{Tr}(H^2) + \text{Tr}(V_k H^2) - \frac{1}{d(d^2 - 1)} \text{Tr}(V_k^2) \text{Tr}(H^2) + \text{Tr}(V_k H^2)\right].
\] (E12)

The integral of the second term in Eq. (E11) can be calculated using Eq. (A4) as follows:
\[
\int dU_L \text{Tr}(U_L V_k^2 U_L^\dagger H^2) = \frac{\text{Tr}(V_k^2) \text{Tr}(H^2)}{d}.
\] (E13)

Finally, after combining everything we get
\[
\text{Var}_{R,L} \partial_k C = -\left(\text{Tr}(\rho^2) - \frac{1}{d}\right) \left(\frac{2}{d^2 - 1}\right) \left(\frac{1}{d^2 - 1}\right) \left[\text{Tr}(V_k^2) \text{Tr}(H^2) + \text{Tr}(V_k H^2)\right]
\]

\[
-\frac{1}{d(d^2 - 1)} \left[\text{Tr}(V_k^2) \text{Tr}(H^2) + \text{Tr}(V_k H^2)\right] - \frac{1}{d} \left[\text{Tr}(V_k^2) \text{Tr}(H^2)\right]
\] (E14)

### F. Numerically studying the correlations between expressibility and cost partial derivatives

In this Appendix we present numerical results on the correlations between the cost gradient and expressibility. Specifically, we consider the layered parametrized ansatz detailed in Section III B of the main text and plot the variance in the PQC gradients as a function of its expressibility.
FIG. 5. Correlations between cost partial derivatives and the state-dependent frame potential. The variance in the partial derivative of a global cost with $H = \prod_{i=1}^n \sigma_i^z$ (top) and 2-local cost with $H = \sigma_1^x \sigma_2^z$ (bottom) as a function of the expressibility measure $\frac{\varphi^{(R)}}{\varphi_{\text{Haar}}^{(R)}}$ (in both cases $\rho = \langle \psi_0 | \psi_0 \rangle^{\otimes n}$ where $|\psi_0\rangle = \exp(-i(\pi/8)\sigma_z)) \rangle$). In the left panel we vary the circuit depth $D$ of a hardware efficient ansatz. In the right (middle) panel we consider the effect of correlating parameters (restricting the directions of rotation) of a hardware efficient ansatz with $D = 100$ with the choices of correlations (rotations) indicated in the figure legend. In all cases $n = 4$, the derivative is taken with respect to $\theta_{ij}$ and the variance and frame potentials are estimating using an ensemble of 5000 unitaries.

We can calculate the expressibility measures $\varepsilon_R^\rho$ and $\varepsilon_R^H$ via their reformulation in terms of the state and Hamiltonian dependent frame potentials $\mathcal{F}_{\text{Haar}}^{(R)} := \mathcal{F}_{\text{Haar}}^{(\rho)}$ and $\mathcal{F}_{\text{Haar}}^{(H)} := \mathcal{F}_{\text{Haar}}^{(L)}$ given in Eq. (B11). However, since it follows from Eq. (B10) that the state (Hamiltonian) dependent frame potential for the Haar distribution $\mathcal{F}_{\text{Haar}}^{(\rho)}$ ($\mathcal{F}_{\text{Haar}}^{(H)}$) is exponentially small, and $\varepsilon_R^\rho$ ($\varepsilon_R^H$) measures the difference between $\mathcal{F}_{\text{Haar}}^{(R)}$ and $\mathcal{F}_{\text{Haar}}^{(\rho)}$ ($\mathcal{F}_{\text{Haar}}^{(H)}$ and $\mathcal{F}_{\text{Haar}}^{(L)}$), it follows that $\varepsilon_R^\rho$ ($\varepsilon_R^H$) may also be exponentially small. We therefore find the ratio of the true frame potential to the Haar frame potential more insightful to plot. That is, we consider the ratios

$$\frac{\mathcal{F}_{\text{Haar}}^{(\rho)}}{\mathcal{F}_{\text{Haar}}^{(R)}} = \frac{(\varepsilon_R^{(\rho)})^2}{\mathcal{F}_{\text{Haar}}^{(\rho)}} + 1$$

$$\frac{\mathcal{F}_{\text{Haar}}^{(H)}}{\mathcal{F}_{\text{Haar}}^{(L)}} = \frac{(\varepsilon_R^{(L)})^2}{\mathcal{F}_{\text{Haar}}^{(H)}} + 1.$$  

(F1)

(F2)

The larger these ratios, the more inexpressive the ansatz, with the ratios tending to 1 for maximally expressive ansätze (exact 2-designs).

In Fig. 5 and Fig. 6 we plot the variance in the partial derivative as a function of $\frac{\varphi^{(R)}}{\varphi_{\text{Haar}}^{(R)}}$ and $\frac{\varphi^{(H)}}{\varphi_{\text{Haar}}^{(H)}}$ respectively. Inline with Section III B of the main text, we focus on three different ways of tuning the expressibility of an ansatz; namely decreasing the depth of the circuits, correlating circuit parameters, and restricting either the direction of rotations. Overall we find a clear correlation between partial derivatives of the cost and expressibility, with the variance in the derivatives increasing with increasing $\frac{\varphi^{(R)}}{\varphi_{\text{Haar}}^{(R)}}$ and $\frac{\varphi^{(H)}}{\varphi_{\text{Haar}}^{(H)}}$.

It is noteworthy that the Hamiltonian dependent frame potential captures the effect of locality on cost gradients as the circuit depth is tuned. As observed in Section III B, increasing the depth of the circuit reduces cost partial derivatives for a local cost but not a global cost. The state dependent frame potential cannot capture this effect since it is independent of the choice in measurement operator $H$ and therefore necessarily independent of the locality of $H$. Conversely, the while the Hamiltonian frame potential for a local cost decreases with increasing depth, inline with the decreasing variance in partial derivatives, the Hamiltonian dependent frame potential for the global cost is effectively constant (even as the depth of the circuit substantially increases) reflecting the effectively constant variance in partial derivatives.

Nonetheless, the correlation between the variance in the cost partial derivative and the expressibility is not perfect, as is clear for example, from Fig. 6(F). This is entirely compatible with our analytical bounds, which are upper bounds and therefore do not enforce perfect correlation between the variance in the partial derivative and the expressibility. Thus while Fig. 5 and Fig. 6 demonstrate a clear correlation between the variance in the partial derivative of the cost...
FIG. 6. Correlations between cost partial derivative and the Hamiltonian-dependent frame potential. This setting here is entirely equivalent to that described in Fig. 5; however, here we plot the variance in the partial derivative as a function of the ratio of Hamiltonian-dependent frame potentials $\frac{F(H)}{F_{\text{Haar}}}$ and the derivative is taken with respect to $\theta_1$.

and expressibility, further work is required to understand the intricacies of this correlation.