Cost-Function-Dependent Barren Plateaus in Shallow Quantum Neural Networks

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Variational quantum algorithms (VQAs) optimize the parameters $\boldsymbol{\theta}$ of a quantum neural network $V(\boldsymbol{\theta})$ to minimize a cost function C. While VQAs may enable practical applications of noisy quantum computers, they are nevertheless heuristic methods with unproven scaling. Here, we rigorously prove two results, assuming $V(\boldsymbol{\theta})$ is a hardware-efficient ansatz composed of blocks forming local 2-designs. Our first result states that defining C in terms of global observables leads to an exponentially vanishing gradient (i.e., a barren plateau) even when $V(\boldsymbol{\theta})$ is shallow. This implies that several VQAs in the literature must revise their proposed cost functions. On the other hand, our second result states that defining C with local observables leads to at worst a polynomially vanishing gradient, so long as the depth of $V(\boldsymbol{\theta})$ is $\mathcal{O}(\log n)$. Taken together, our results establish a connection between locality and trainability. Finally, we illustrate these ideas with large-scale simulations, up to 100 qubits, of a particular VQA known as quantum autoencoders.

I. Introduction

One of the most important technological questions is whether Noisy Intermediate-Scale Quantum (NISQ) computers will have practical applications [1]. NISQ devices are limited both in qubit count and in gate fidelity, hence preventing the use of quantum error correction.

The leading strategy to make use of these devices are variational quantum algorithms (VQAs) [2]. VQAs employ a quantum computer to efficiently evaluate a cost function C, while a classical optimizer trains the parameters θ of a parameterized quantum circuit $V(\theta)$. The latter represents a quantum generalization of a neural network, i.e., a quantum neural network (QNN). The benefits of VQAs are three-fold. First, VQAs allow for task-oriented programming of quantum computers, which is important since designing quantum algorithms is non-intuitive. Second, VQAs make up for small qubit counts by leveraging classical computational power. Third, pushing complexity onto classical computers, while only running short-depth quantum circuits, is an effective strategy for error mitigation on NISQ devices.

There are very few rigorous scaling results for VQAs (with one-layer approximate optimization being an exception [3–5]). Ideally one would like to employ a hardware-efficient ansatz [6] for $V(\theta)$, but one of the few known scaling results is that deep versions of such ansatzes lead to vanishing gradients [7]. Very little is known about the trainability of such ansatzes for shallow depths, and it would be especially useful to have a converse bound that guarantees trainability for certain depths. This motivates our work, where we rigorously investigate the trainability of VQAs as a function of the circuit depth.

The other motivation for our work is the recent explosion in the number of proposed VQAs. The Variational Quantum Eigensolver (VQE) is the most famous VQA. It aims to prepare the ground state of a given Hamiltonian $H = \sum_{\alpha} c_{\alpha} \sigma_{\alpha}$, with H expanded as a sum of local Pauli operators [8]. In VQE, the cost function is

obviously the energy $C=\langle\psi|H|\psi\rangle$ of the trial state $|\psi\rangle$. However, VQAs have been proposed for other applications, like quantum data compression [9], quantum error correction [10], quantum metrology [11], quantum compiling [12–15], quantum state diagonalization [16, 17], quantum simulation [18–21], fidelity estimation [22], unsampling [23], consistent histories [24], and linear systems [25–27]. For these applications, the choice of C is less obvious. Put another way, if one reformulates these VQAs as ground-state problems (which can be done in many cases), the choice of Hamiltonian H is less intuitive. This is because many of these applications are abstract, rather than associated with a physical Hamiltonian.

Here we connect the trainability of VQAs to the choice of C. For the abstract applications in Refs. [9–27], it is important for C to be operational, so that small values of C imply that the task is almost accomplished. Consider an example of state preparation, where the goal is to find a gate sequence that prepares a target state $|\psi_0\rangle$. A natural cost function is the square of the trace distance D_T between $|\psi_0\rangle$ and $|\psi\rangle = V(\theta)^{\dagger}|0\rangle$, given by $C_G = D_T(|\psi_0\rangle, |\psi\rangle)^2$, which is equivalent to

$$C_G = \text{Tr}[O_G V(\boldsymbol{\theta})|\psi_0\rangle\langle\psi_0|V(\boldsymbol{\theta})^{\dagger}], \qquad (1)$$

with $O_G = 1 - |\mathbf{0}\rangle\langle\mathbf{0}|$. Note that $\sqrt{C_G} \geqslant |\langle\psi|M|\psi\rangle - \langle\psi_0|M|\psi_0\rangle|$ has a nice operational meaning as a bound on the expectation value difference for a POVM element M.

However, we argue that this cost function and others like it are untrainable due to a vanishing gradient. Namely, we consider global cost functions, where one directly compares states or operators living in exponentially large Hilbert spaces (e.g., $|\psi\rangle$ and $|\psi_0\rangle$). These are precisely the cost functions that have operational meanings for tasks of interest, including all tasks in Refs. [9–27]. Hence, our results imply that a non-trivial subset of these references will need to revise their choice of C.

Interestingly, we demonstrate vanishing gradients for shallow QNNs. This is in contrast to McClean et al. [7], who showed vanishing gradients for deep QNNs. They noted that randomly initializing θ for a $V(\theta)$ that forms a 2-design leads to a barren plateau, i.e., with the gradient

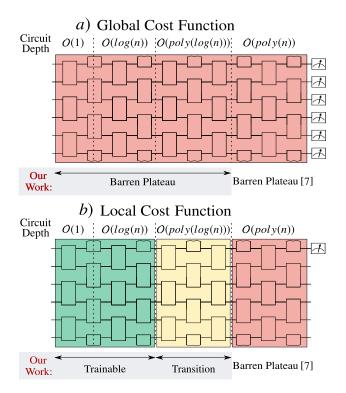


FIG. 1. Summary of our main results. McClean et al. [7] proved that a barren plateau can occur when the depth D of a hardware-efficient ansatz is $D \in \mathcal{O}(\operatorname{poly}(n))$. Here we extend these results by providing bounds for the variance of the gradient of global and local cost functions as a function of D. In particular, we find that the barren plateau phenomenon is cost-function dependent. a) For global cost functions (e.g., Eq. (1)), the landscape will exhibit a barren plateau essentially for all depths D. b) For local cost functions (e.g., Eq. (2)), the gradient vanishes at worst polynomially and hence is trainable when $D \in \mathcal{O}(\log(n))$, while barren plateaus occur for $D \in \mathcal{O}(\operatorname{poly}(n))$, and between these two regions the gradient transitions from polynomial to exponential decay.

vanishing exponentially in the number of qubits, n. Their work implied that researchers must develop either clever parameter initialization strategies [28, 29] or clever QNN ansatzes [4, 30, 31]. Similarly, our work implies that researchers must carefully weigh the balance between trainability and operational relevance when choosing C.

While our work is for general VQAs, barren plateaus for global cost functions were noted for specific VQAs and for a very specific tensor-product example by our research group [12, 16], and more recently in [27]. This motivated the proposal of local cost functions [12, 14, 16, 20, 23–25], where one compares objects (states or operators) with respect to each individual qubit, rather than in a global sense, and therein it was shown that these local cost functions have indirect operational meaning.

Our second result is that these local cost functions have gradients that vanish polynomially rather than exponentially in n, and hence have the potential to be trained. This holds for $V(\theta)$ with depth $\mathcal{O}(\log n)$. Figure 1 summarizes our two main results.

Finally, we illustrate these ideas for an important example: quantum autoencoders [9]. Our large-scale numerics show that the global cost function proposed in [9] is untrainable for large n. On the other hand, we propose a novel local cost function that is trainable, hence making quantum autoencoders a scalable application.

II. Results

A. Warm-up example

To illustrate cost-function-dependent barren plateaus, we first consider a toy problem corresponding to the state preparation problem in the Introduction with the target state being $|\mathbf{0}\rangle$. We assume a tensor-product ansatz of the form $V(\boldsymbol{\theta}) = \bigotimes_{j=1}^n e^{-i\theta^j \sigma_x^{(j)}/2}$, with the goal of finding the angles θ^j such that $V(\boldsymbol{\theta})|\mathbf{0}\rangle = |\mathbf{0}\rangle$. Employing the global cost of (1) results in $C_G = 1 - \prod_{j=1}^n \cos^2 \frac{\theta^j}{2}$. The barren plateau can be detected via the variance of its gradient: $\operatorname{Var}\left[\frac{\partial C_G}{\partial \theta^j}\right] = \frac{1}{8}(\frac{3}{8})^{n-1}$, which is exponentially vanishing in n. Since the mean value is $\langle \frac{\partial C_G}{\partial \theta^j} \rangle = 0$, the gradient concentrates exponentially around zero.

On the other hand, consider a local cost function:

$$C_L = \text{Tr} \left[O_L V(\boldsymbol{\theta}) | \mathbf{0} \rangle \langle \mathbf{0} | V(\boldsymbol{\theta})^{\dagger} \right],$$
 (2)

with
$$O_L = \mathbb{1} - \frac{1}{n} \sum_{j=1}^n |0\rangle\langle 0|_j \otimes \mathbb{1}_{\overline{j}},$$
 (3)

where $1_{\bar{j}}$ is the identity on all qubits except qubit j. Note that C_L vanishes under the same conditions as C_G [12, 14], $C_L = 0 \Leftrightarrow C_G = 0$. We find $C_L = 1 - \frac{1}{n} \sum_{j=1}^n \cos^2 \frac{\theta^j}{2}$, and the variance of its gradient is $\mathrm{Var}[\frac{\partial C_L}{\partial \theta^j}] = \frac{1}{8n^2}$, which vanishes polynomially with n and hence exhibits no barren plateau. Figure 2 depicts the cost landscapes of C_G and C_L for two values of n and shows that the barren plateau can be avoided here via a local cost function.

Moreover, this example allows us to delve deeper into the cost landscape to see a phenomenon that we refer to as a narrow gorge. While a barren plateau is associated with a flat landscape, a narrow gorge refers to the steepness of the valley that contains the global minimum. This phenomenon is illustrated in Fig. 2, where each dot corresponds to cost values obtained from randomly selected parameters $\boldsymbol{\theta}$. For C_G we see that very few dots fall inside the narrow gorge, while for C_L the narrow gorge is not present. Note that the narrow gorge makes it harder to train C_G since the learning rate of descent-based optimization algorithms must be exponentially small in order not to overstep the narrow gorge. The following proposition (proved in the Supplementary Information) formalizes the narrow gorge for C_G and its absence for C_L by bounding the probability that $C \leq \delta$ for a given δ . This probability is associated with the parameter space volume that leads to $C \leq \delta$.

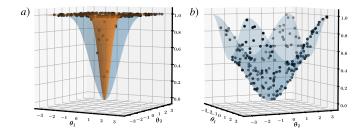


FIG. 2. Cost function landscapes. a) Two-dimensional cross-section through the landscape of $C_G = 1 - \prod_{j=1}^n \cos^2(\theta^j/2)$ for n=4 (blue) and n=24 (orange). b) The same cross-section through the landscape of $C_L = 1 - \frac{1}{n} \sum_{j=1}^n \cos^2(\theta^j/2)$ is independent of n. In both cases, 200 Haar distributed points are shown, with very few (most) of these points lying in the valley containing the global minimum of C_G (C_L).

Proposition 1. If θ^j is uniformly distributed on $[-\pi, \pi]$ $\forall j$, then for any $\delta \in (0,1)$, and in the limit that n is large, the probability that $C_G \leq \delta$ is upper bounded by

$$\Pr\left\{C_G \leqslant \delta \mid \forall \delta \in (0,1)\right\} \leqslant \frac{\left(2\pi e\left(1 - \left(1 - \delta\right)^{\frac{1}{n}}\right)\right)^{\frac{n}{2}}}{\sqrt{\pi n}}.$$
 (4)

For $\delta \in (1/2,1]$, the probability that $C_L \leq \delta$ is lower bounded by

$$\Pr\left\{C_L \leqslant \delta \mid \forall \delta \in (1/2, 1]\right\} \geqslant \frac{(2\delta - 1)^2}{(2\delta - 1)^2 + \frac{1}{2n}} \xrightarrow[n \to \infty]{} 1. \quad (5)$$

B. General framework

1. General cost function

For our general results, we consider a family of cost functions that can be expressed as the expectation value of an operator O as follows

$$C = \text{Tr} \left[OV(\boldsymbol{\theta}) \rho V^{\dagger}(\boldsymbol{\theta}) \right] , \qquad (6)$$

where ρ is an arbitrary quantum state on n qubits. Note that this framework includes the special case where ρ could be a pure state, as well as the more special case where $\rho = |\mathbf{0}\rangle\langle\mathbf{0}|$, which is the input state for many VQAs such as VQE. Moreover, in VQE, one chooses O = H, where H is the physical Hamiltonian. In general, the choice of O and ρ essentially defines the application of interest of the particular VQA.

It is typical to express O as a linear combination of the form $O = c_0 \mathbb{1} + \sum_{i=1}^N c_i O_i$. Here $O_i \neq \mathbb{1}$, $c_i \in \mathbb{R}$, and we assume that at least one $c_i \neq 0$. Note that C_G and C_L in (1) and (2) fall under this framework. In our main results below, we will consider two different choices of O that respectively capture our general notions of global and local cost functions and also generalize the aforementioned C_G and C_L .

2. Ansatz

Our general results employ a layered hardware-efficient ansatz [6]. This choice of ansatz reduces gate overhead that arises when implementing on quantum hardware. As shown in Fig. 3(a), $V(\theta)$ consists of L layers of m-qubit gates $W_{kl}(\theta_{kl})$, or blocks, acting on alternating groups of m neighboring qubits. We refer to this as an Alternating Layered Ansatz. Here we assume for simplicity that L is odd, although our results can be generalized for the case when L is even. The index $l=1,\ldots,L$ in $W_{kl}(\theta_{kl})$ indicates the layer that contains the block, while $k=1,\ldots,\xi$ indicates the qubits it acts upon. We assume n is a multiple of m, with $n=m\xi$, and that m does not scale with n.

Without loss of generality, any block $W_{kl}(\boldsymbol{\theta}_{kl})$ can be written as a product of ζ_{kl} independent gates from a gate alphabet $\mathcal{A} = \{G_u(\boldsymbol{\theta})\}$ as

$$W_{kl}(\boldsymbol{\theta}_{kl}) = G_{\zeta_{kl}}(\boldsymbol{\theta}_{kl}^{\zeta_{kl}}) \dots G_{\nu}(\boldsymbol{\theta}_{kl}^{\nu}) \dots G_{1}(\boldsymbol{\theta}_{kl}^{1}), \quad (7)$$

where each θ_{kl}^{ν} is a continuous parameter. Here, $G_{\nu}(\theta_{kl}^{\nu}) = R_{\nu}(\theta_{kl}^{\nu})Q_{\nu}$ where Q_{ν} is an unparameterized gate and $R_{\nu}(\theta_{kl}^{\nu}) = e^{-i\theta_{kl}^{\nu}\sigma_{\nu}/2}$ with σ_{ν} a Pauli operator. Note that W_{kL} denotes a block in the last layer of $V(\theta)$. As depicted in Fig. 3(a), we define S_k as the m-qubit subsystem on which W_{kL} acts, and we define $S = \{S_k\}$ as the set of all such subsystems.

For the proofs of our results, it is helpful to conceptually break up the ansatz as follows. Consider a block $W_{kl}(\theta_{kl})$ in the l-th layer of the ansatz. For simplicity we henceforth use W to refer to a given $W_{kl}(\theta_{kl})$. Let S_w denote the m-qubit subsystem that contains the qubits W acts on, and let $S_{\overline{w}}$ be the (n-m) subsystem on which W acts trivially. Similarly, let \mathcal{H}_w and $\mathcal{H}_{\overline{w}}$ denote the Hilbert spaces associated with S_w and $S_{\overline{w}}$, respectively. Then, as shown in Fig. 3(a), $V(\theta)$ can be expressed as

$$V(\boldsymbol{\theta}) = V_L(\mathbb{1}_{\overline{w}} \otimes W) V_R. \tag{8}$$

Here, $\mathbb{1}_{\overline{w}}$ is the identity on $\mathcal{H}_{\overline{w}}$, and V_R contains the gates in the (forward) light-cone \mathcal{L} of W, i.e., all gates with at least one input qubit causally connected to the output qubits of W. The latter allows us to define $S_{\mathcal{L}}$ as the subsystem of all qubits in \mathcal{L} .

3. Gradient of the cost function

The contribution to the gradient ∇C from a parameter θ^{ν} is given by the partial derivative $\frac{\partial C}{\partial \theta^{\nu}} := \partial_{\nu} C$. Assuming that θ^{ν} is a parameter inside a given block W, we obtain from (6), (7), and (8)

$$\partial_{\nu}C = \frac{i}{2} \operatorname{Tr} \left[(\mathbb{1}_{\overline{w}} \otimes W_B) V_L \rho V_L^{\dagger} (\mathbb{1}_{\overline{w}} \otimes W_B^{\dagger}) \right]$$
 (9)

$$\times \left[\mathbb{1}_{\overline{w}} \otimes \sigma_{\nu}, (\mathbb{1}_{\overline{w}} \otimes W_A^{\dagger}) V_R^{\dagger} O V_R (\mathbb{1}_{\overline{w}} \otimes W_A)\right] ,$$

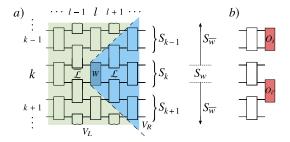


FIG. 3. Alternating Layered Ansatz. a) Each block W_{kl} acts on m qubits and is parameterized via (7). As shown, we define S_k as the m-qubit subsystem on which W_{kL} acts, where L is the last layer of $V(\boldsymbol{\theta})$. Given some block W, it is useful for our proofs (outlined in the Methods) to write $V(\boldsymbol{\theta}) = V_L(\mathbb{1}_{\overline{w}} \otimes W)V_R$, where V_R contains all gates in the forward light-cone \mathcal{L} of W. The forward light-cone \mathcal{L} is defined as all gates with at least one input qubit causally connected to the output qubits of W. We define $\overline{\mathcal{L}}$ as the compliment of \mathcal{L} , S_w as the m-qubit subsystem on which W acts, and $S_{\overline{w}}$ as the n-m qubit subsystem on which W acts trivially. b) The operator O_i acts non-trivially only in subsystem $S_{k-1} \in \mathcal{S}$, while $O_{i'}$ acts non-trivially on the first m/2 qubits of S_{k+1} , and on the second m/2 qubits of S_k .

with

$$W_B = \prod_{\mu=1}^{\nu-1} G_{\mu}(\theta^{\mu}), \text{ and } W_A = \prod_{\mu=\nu}^{\zeta} G_{\mu}(\theta^{\mu}).$$
 (10)

While the value of $\partial_{\nu}C$ depends on the specific parameters $\boldsymbol{\theta}$, it is useful to compute $\langle \partial_{\nu}C \rangle_{V}$, i.e., the average gradient over all possible unitaries $V(\boldsymbol{\theta})$ within the ansatz. Such an average may not be representative near the minimum of C, although it does provide a good estimate of the expected gradient when randomly initializing the angles in $V(\boldsymbol{\theta})$. In the Methods Section we explicitly show how to compute averages of the form $\langle \dots \rangle_{V}$, and in the Supplementary Information we provide a proof for the following Proposition.

Proposition 2. The average of the partial derivative of any cost function of the form (6) with respect to a parameter θ^{ν} in a block W of the ansatz in Fig. 3 is

$$\langle \partial_{\nu} C \rangle_{V} = 0, \qquad (11)$$

provided that either W_A or W_B of (10) form a 1-design.

Here we recall that a t-design is an ensemble of unitaries, such that sampling over their distribution yields the same properties as sampling random unitaries from the unitary group with respect to the Haar measure up to the first t moments [32]. The Methods section provides a formal definition of a t-design.

Proposition 2 states that the gradient is not biased in any particular direction. To analyze the trainability of C, one must also consider the second moment of its partial derivatives:

$$\operatorname{Var}[\partial_{\nu}C] = \left\langle \left(\partial_{\nu}C\right)^{2}\right\rangle_{V}, \qquad (12)$$

where we used the fact that $\langle \partial_{\nu} C \rangle_{V} = 0$. The magnitude of $\operatorname{Var}[\partial_{\nu} C]$ quantifies how much the partial derivative concentrates around zero, and hence small values in (12) imply that the slope of the landscape will typically be insufficient to provide a cost-minimizing direction. Specifically, from Chebyshev's inequality, $\operatorname{Var}[\partial_{\nu} C]$ bounds the probability that the cost-function partial derivative deviates from its mean value (of zero) as

$$\Pr(|\partial_{\nu}C| \geqslant c) \leqslant \frac{\operatorname{Var}[\partial_{\nu}C]}{c^2}, \quad \forall c > 0.$$
 (13)

We derive a general formula for the variance:

$$\operatorname{Var}[\partial_{\nu}C] = \frac{2^{m-1}\operatorname{Tr}[\sigma_{\nu}^{2}]}{(2^{2m}-1)^{2}} \sum_{\substack{pq \ p'q'}} \langle \Delta\Omega_{qp}^{q'p'} \rangle_{V_{R}} \langle \Delta\Psi_{pq}^{p'q'} \rangle_{V_{L}} \quad (14)$$

which holds if W_A and W_B form independent 2-designs. Here, the summation runs over all bistrings p, q, p', q' of length 2^{n-m} . In addition, we defined

$$\Delta\Omega_{\boldsymbol{qp}}^{\boldsymbol{q'p'}} = \text{Tr}[\Omega_{\boldsymbol{qp}}\Omega_{\boldsymbol{q'p'}}] - \frac{\text{Tr}[\Omega_{\boldsymbol{qp}}]\text{Tr}[\Omega_{\boldsymbol{q'p'}}]}{2^m}, \qquad (15)$$

$$\Delta \Psi_{\boldsymbol{p}\boldsymbol{q}}^{\boldsymbol{p}'\boldsymbol{q}'} = \text{Tr}[\Psi_{\boldsymbol{p}\boldsymbol{q}}\Psi_{\boldsymbol{p}'\boldsymbol{q}'}] - \frac{\text{Tr}[\Psi_{\boldsymbol{p}\boldsymbol{q}}]\text{Tr}[\Psi_{\boldsymbol{p}'\boldsymbol{q}'}]}{2^m}, \quad (16)$$

where $\text{Tr}_{\overline{w}}$ indicates the trace over subsystem $S_{\overline{w}}$, and Ω_{qp} and Ψ_{qp} are operators on \mathcal{H}_w defined as

$$\Omega_{qp} = \text{Tr}_{\overline{w}} \left[(|p\rangle \langle q| \otimes \mathbb{1}_w) V_R^{\dagger} O V_R \right] , \qquad (17)$$

$$\Psi_{pq} = \operatorname{Tr}_{\overline{w}} \left[(|\boldsymbol{q}\rangle\langle \boldsymbol{p}| \otimes \mathbb{1}_w) V_L \rho V_L^{\dagger} \right] . \tag{18}$$

We derive Eq. (14) in the Supplementary Information.

C. Main results

Here we present our main theorems and corollaries, with the proofs sketched in the Methods and detailed in the Supplementary Information. In addition, in the Supplementary Information we analyze a generalization of the warm-up example where ρ is arbitrary, and where $V(\theta)$ is composed of a single layer of the ansatz in Fig. 3. This case bridges the gap between the warm-up example and our main theorems and also showcases the tools used to derive our main result.

The following theorem provides an upper bound on the variance of the partial derivative of a global cost function which can be expressed as the expectation value of an operator of the form

$$O = c_0 \mathbb{1} + \sum_{i=1}^{N} c_i \widehat{O}_{i1} \otimes \widehat{O}_{i2} \otimes \cdots \otimes \widehat{O}_{i\xi}.$$
 (19)

Specifically, we consider two cases of interest: (i) When N=1 and each \widehat{O}_{1k} is a non-trivial projector ($\widehat{O}_{1k}^2=\widehat{O}_{1k}\neq \mathbb{1}$) of rank r_k acting on subsystem S_k , or (ii) When

N is arbitrary and \widehat{O}_{ik} is traceless with $\text{Tr}[\widehat{O}_{ik}^2] \leq 2^m$ (for example, when $\widehat{O}_{ik} = \bigotimes_{j=1}^m \sigma_j^\mu$ is a tensor product of Pauli operators $\sigma_j^\mu \in \{\mathbb{1}_j, \sigma_j^x, \sigma_j^y, \sigma_j^z\}$, with at least one $\sigma_j^\mu \neq \mathbb{1}$). Note that case (i) includes C_G of (1) as a special case.

Theorem 1. Consider a trainable parameter θ^{ν} in a block W of the ansatz in Fig. 3. Let $Var[\partial_{\nu}C]$ be the variance of the partial derivative of a global cost function C (with O given by (19)) with respect to θ^{ν} . If each block in $V(\theta)$ forms a local 2-design, then $Var[\partial_{\nu}C]$ is upper bounded by

$$Var[\partial_{\nu}C] \leqslant F_n(L,l). \tag{20}$$

(i) For N=1 and when each \widehat{O}_{1k} is a non-trivial projector, then defining $R=\prod_{k=1}^{\xi}r_k^2$, we have

$$F_n(L,l) = \frac{2^{2m + (2m-1)(L-l)}}{(2^{2m} - 1) \cdot 3^{\frac{n}{m}} \cdot 2^{(2-\frac{3}{m})n}} c_1^2 R.$$
 (21)

(ii) For arbitrary N and when each \widehat{O}_{ik} satisfies $\operatorname{Tr}[\widehat{O}_{ik}] = 0$ and $\operatorname{Tr}[\widehat{O}_{ik}^2] \leqslant 2^m$, then

$$F_n(L,l) = \frac{2^{2m(L-l+1)+1}}{3^{\frac{2n}{m}} \cdot 2^{\left(3-\frac{4}{m}\right)n}} \sum_{i,j=1}^{N} c_i c_j.$$
 (22)

From Theorem 1 we derive the following corollary.

Corollary 1. Consider the function $F_n(L, l)$.

(i) Let N=1 and let each \widehat{O}_{1k} be a non-trivial projector, as in case (i) of Theorem 1. If $c_1^2R \in \mathcal{O}(2^n)$ and if the number of layers $L \in \mathcal{O}(\operatorname{poly}(\log(n)))$, then

$$F_n(L,l) \in \mathcal{O}\left(2^{-\left(1-\frac{1}{m}\log_2 3\right)n}\right),$$
 (23)

which implies that $\operatorname{Var}[\partial_{\nu}C]$ is exponentially vanishing in n if $m \ge 2$.

(ii) Let N be arbitrary, and let each \widehat{O}_{ik} satisfy $\operatorname{Tr}[\widehat{O}_{ik}] = 0$ and $\operatorname{Tr}[\widehat{O}_{ik}^2] \leqslant 2^m$, as in case (ii) of Theorem 1. If $N \in \mathcal{O}(2^n)$, $c_i \in \mathcal{O}(1)$, and if the number of layers $L \in \mathcal{O}(\operatorname{poly}(\log(n)))$, then

$$F_n(L,l) \in \mathcal{O}\left(\frac{1}{2(1-\frac{1}{m})n}\right),$$
 (24)

which implies that $Var[\partial_{\nu}C]$ is exponentially vanishing in n if $m \ge 2$.

Let us now make several important remarks. First, note that part (i) of Corollary 1 includes as a particular example the cost function C_G of (1). Second, part (ii) of this corollary also includes as particular examples operators with $N \in \mathcal{O}(1)$, as well as $N \in \mathcal{O}(\text{poly}(n))$. Finally, we remark that $F_n(L, l)$ becomes trivial when the number

of layers L is $\mathcal{O}(\text{poly}(n))$, however, as we discuss below, we can still find that $\text{Var}[\partial_{\nu}C_G]$ vanishes exponentially in this case.

Our second main theorem shows that barren plateaus can be avoided for shallow circuits by employing local cost functions. Here we consider m-local cost functions where each \widehat{O}_i acts non-trivially on at most m qubits and (on these qubits) can be expressed as $\widehat{O}_i = \widehat{O}_i^{\mu_i} \otimes \widehat{O}_i^{\mu'_i}$:

$$O = c_0 \mathbb{1} + \sum_{i=1}^{N} c_i \widehat{O}_i^{\mu_i} \otimes \widehat{O}_i^{\mu'_i}, \qquad (25)$$

where $\widehat{O}_i^{\mu_i}$ are operators acting on m/2 qubits which can be written as a tensor product of Pauli operators. Here, we assume the summation in Eq. (25) includes two possible cases as schematically shown in Fig. 3(b): First, when $\widehat{O}_i^{\mu_i}$ ($\widehat{O}_i^{\mu_i'}$) acts on the first (last) m/2 qubits of a given S_k , and second, when $\widehat{O}_i^{\mu_i}$ ($\widehat{O}_i^{\mu_i'}$) acts on the last (first) m/2 qubits of a given S_k (S_{k+1}). This type of cost function includes any ultralocal cost function (i.e., where the \widehat{O}_i are one-body) as in (2), and also VQE Hamiltonians with up to m/2 neighbor interactions. Then, the following theorem holds.

Theorem 2. Consider a trainable parameter θ^{ν} in a block W of the ansatz in Fig. 3. Let $Var[\partial_{\nu}C]$ be the variance of the partial derivative of an m-local cost function C (with O given by (25)) with respect to θ^{ν} . If each block in $V(\theta)$ forms a local 2-design, then $Var[\partial_{\nu}C]$ is lower bounded by

$$G_n(L, l) \leqslant \operatorname{Var}[\partial_{\nu} C],$$
 (26)

with

$$G_n(L,l) = \frac{2^{m(l+1)-1}}{(2^{2m}-1)^2(2^m+1)^{L+l}} \times \sum_{\substack{i \in i_{\mathcal{L}} \\ k' \geqslant k}} \sum_{\substack{c_i^2 \in (\rho_{k,k'}) \in (\widehat{O}_i), \\ k' \geqslant k}} c_i^2 \epsilon(\rho_{k,k'}) \epsilon(\widehat{O}_i), \qquad (27)$$

where $i_{\mathcal{L}}$ is the set of i indices whose associated operators \widehat{O}_i act on qubits in the forward light-cone \mathcal{L} of W, and $k_{\mathcal{L}_B}$ is the set of k indices whose associated subsystems S_k are in the backward light-cone \mathcal{L}_B of W. Here we defined the function $\epsilon(M) = D_{HS}(M, \operatorname{Tr}(M) \mathbb{1}/d_M)$ where D_{HS} is the Hilbert-Schmidt distance and d_M is the dimension of the matrix M. In addition, $\rho_{k,k'}$ is the partial trace of the input state ρ down to the subsystems $S_k S_{k+1}...S_{k'}$.

Let us make a few remarks. First, note that the $\epsilon(\widehat{O}_i)$ in the lower bound indicates that training $V(\boldsymbol{\theta})$ is easier when \widehat{O}_i is far from the identity. Second, the presence of $\epsilon(\rho_{k,k'})$ in $G_n(L,l)$ implies that we have no guarantee on the trainability of a parameter θ^{ν} in W if ρ is maximally mixed on the qubits in the backwards light-cone.

From Theorem 2 we derive the following corollary for m-local cost functions, which guarantees the trainability of the ansatz for shallow circuits.

Corollary 2. Consider the function $F_n(L, l)$. Let O be an operator of the form (25), as in Theorem 2. If at least one term $c_i^2 \epsilon(\rho_{k,k'}) \epsilon(\widehat{O}_i)$ in the sum in (27) vanishes no faster than $\Omega(1/\operatorname{poly}(n))$, and if the number of layers L is $\mathcal{O}(\log(n))$, then

$$G_n(L,l) \in \Omega\left(\frac{1}{\text{poly}(n)}\right)$$
 (28)

On the other hand, if at least one term $c_i^2 \epsilon(\rho_{k,k'}) \epsilon(\widehat{O}_i)$ in the sum in (27) vanishes no faster than $\Omega\left(1/2^{\operatorname{poly}(\log(n))}\right)$, and if the number of layers is $\mathcal{O}(\operatorname{poly}(\log(n)))$, then

$$G_n(L,l) \in \Omega\left(\frac{1}{2^{\text{poly}(\log(n))}}\right)$$
 (29)

Hence, when L is $\mathcal{O}(\text{poly}(\log(n)))$ there is a transition region where the lower bound vanishes faster than polynomially, but slower than exponentially.

We finally justify the assumption of each block being a local 2-designs as follows. It has been shown that one-dimensional 2-designs have efficient quantum circuit descriptions, requiring depths of $\mathcal{O}(m^2)$ gates to be exactly implemented [32], or depth $\mathcal{O}(m)$ to be approximately implemented [33, 34]. Hence, an L-layered ansatz in which each block forms a 2-design can be exactly implemented with a depth $D \in \mathcal{O}(m^2L)$, and approximately implemented with $D \in \mathcal{O}(mL)$.

Moreover, in [34] it has been shown that the Alternating Layered Ansatz of Fig. 3 will form an approximate one-dimensional 2-design on n qubits if the number of layers is $\mathcal{O}(n)$. Hence, for deep circuits, our ansatz behaves like a random circuit and we recover the barren plateaus of [7] for both local and global cost functions.

D. Numerical simulations

As an important example to illustrate the costfunction-dependent barren plateau phenomenon, we consider quantum autoencoders [9, 35–38]. In particular, the pioneering VQA proposed in Ref. [9] has received significant literature attention, due to its importance to quantum machine learning and quantum data compression. Let us briefly explain the algorithm in Ref. [9].

1. Quantum autoencoder

Consider a bipartite quantum system AB composed of n_A and n_B qubits, respectively, and let $\{p_\mu, |\psi_\mu\rangle\}$ be an ensemble of pure states on AB. The goal of the quantum autoencoder is to train a gate sequence $V(\theta)$ to compress this ensemble into the A subsystem, such that one can recover each state $|\psi_\mu\rangle$ with high fidelity from the information in subsystem A. One can think of B as the "trash" since it is discarded after the action of $V(\theta)$. As noted in [9], there is a close connection between data compression

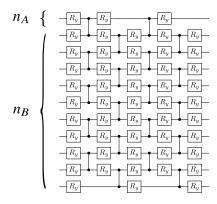


FIG. 4. Alternating Layered Ansatz for $V(\theta)$ employed in our numerical simulations. Each layer is composed of control-Z gates acting on alternating pairs of neighboring qubits which are preceded and followed by single qubit rotations around the y-axis, $R_y(\theta_i) = e^{-i\theta_i\sigma_y/2}$. Shown is the case of two layers, $n_A = 1$, and $n_B = 10$ qubits. The number of variational parameters and gates scales linearly with n_B : for the case shown there are 71 gates and 51 parameters.

and decoupling. Namely, if the subsystem B can be perfectly decoupled from AB then the autoencoder reaches lossless compression. For example, if the output of the B system is a fixed pure state, say $|\mathbf{0}\rangle$, independent of the index μ , then B is decoupled from A and consequently the ensemble has been successfully compressed into A.

To quantify the degree of decoupling (hence data compression), Ref. [9] proposed a cost function of the form:

$$C_G' = 1 - \text{Tr}[|\mathbf{0}\rangle\langle\mathbf{0}|\rho_B^{\text{out}}] \tag{30}$$

$$= \operatorname{Tr}[O'_{G}V(\boldsymbol{\theta})\rho_{AB}^{\mathrm{in}}V(\boldsymbol{\theta})^{\dagger}], \qquad (31)$$

where $\rho_{AB}^{\rm in} = \sum_{\mu} p_{\mu} |\psi_{\mu}\rangle\langle\psi_{\mu}|$ is the ensemble-average input state, $\rho_{B}^{\rm out} = \sum_{\mu} p_{\mu} {\rm Tr}_{A}[|\psi_{\mu}'\rangle\langle\psi_{\mu}'|]$ is the ensemble-average trash state, and $|\psi_{\mu}'\rangle = V(\theta)|\psi_{\mu}\rangle$. Equation (31) makes it clear that C_{G}' has the form in (6), and $O_{G}' = \mathbb{1}_{AB} - \mathbb{1}_{A} \otimes |\mathbf{0}\rangle\langle\mathbf{0}|$ is a global observable of the form in (19). Hence, according to Corollary 1, C_{G}' exhibits a barren plateau for large n_{B} . (Specifically, Corollary 1 applies in this context when $n_{A} < n_{B}$). As a result, large-scale data compression, where one is interested in discarding large numbers of qubits, will not be possible with the C_{G}' cost function.

To address this issue, we propose the following local cost function

$$C'_{L} = 1 - \frac{1}{n_{B}} \sum_{j=1}^{n_{B}} \operatorname{Tr}\left[\left(|0\rangle\langle 0|_{j} \otimes \mathbb{1}_{\overline{j}}\right) \rho_{B}^{\operatorname{out}}\right]$$
(32)

$$= \text{Tr}[O_L'V(\boldsymbol{\theta})\rho_{AB}^{\text{in}}V(\boldsymbol{\theta})^{\dagger}], \qquad (33)$$

where $O'_L = \mathbbm{1}_{AB} - \frac{1}{n_B} \sum_{j=1}^{n_B} \mathbbm{1}_A \otimes |0\rangle\langle 0|_j \otimes \mathbbm{1}_{\overline{j}}$, and $\mathbbm{1}_{\overline{j}}$ is the identity on all qubits in B except the j-th qubit. As shown in the Supplementary Information, C'_L satisfies $C'_L \leqslant C'_G \leqslant n_B C'_L$, which implies that C'_L is faithful (vanishing under the same conditions as C'_G). Further-

more, note that O'_L has the form in (25). Hence Corollary 2 implies that C'_L does not exhibit a barren plateau for shallow ansatzes.

In our heuristics, we simulate the autoencoder algorithm to solve a simple problem where $n_A = 1$, and where the input state ensemble $\{p_{\mu}, |\psi_{\mu}\rangle\}$ is given by

$$|\psi_1\rangle = |0\rangle_A \otimes |0, 0, 0, \dots, 0\rangle_B$$
, with $p_1 = 2/3$, (34)
 $|\psi_2\rangle = |1\rangle_A \otimes |1, 1, 0, \dots, 0\rangle_B$, with $p_2 = 1/3$. (35)

In order to analyze the cost-function-dependent barren plateau phenomenon, the dimension of subsystem B is gradually increased as $n_B = 10, 15, \ldots, 100$.

2. Ansatz and optimization method

The trainable gate sequence $V(\theta)$ is given by two layers of the ansatz in Fig. 4, so that the number of gates and parameters in $V(\theta)$ increases linearly with n_B . Note that this ansatz is a simplified version of the ansatz in Fig. 3, as we can only generate unitaries with real coefficients. While each block in this ansatz will not form an exact local 2-design, and hence does not fall under our theorems, one can still obtain a cost-function-dependent barren plateau as we discuss below.

Let us now describe the optimization method employed to train the gate sequence $V(\theta)$ and minimize the cost functions. First, we note that all the parameters in the ansatz are randomly initialized. Then, at each iteration, one solves the following sub-space search problem: $\min_{\boldsymbol{s} \in \mathbb{R}^d} C(\boldsymbol{\theta} + \boldsymbol{A} \cdot \boldsymbol{s})$, where \boldsymbol{A} is a randomly generated isometry, and $\mathbf{s} = (s_1, \dots, s_d)$ is a vector of coefficients to be optimized over. We used d = 10 in our simulations. Moreover, the training algorithm gradually increases the number of shots per cost-function evaluation. Initially, C is evaluated with 10 shots, and once the optimization reaches a plateau, the number of shots is increased by a factor of 3/2. This process is repeated until a termination condition on the value of C is achieved, or until we reach the maximum value of 10⁵ shots per function evaluation. We also remark that a more advanced measurement-frugal gradient-descent based optimization method can be found in Ref. [39].

3. Numerical results

Figure 5 shows representative results of our numerical implementations of the quantum autoencoder in Ref. [9] obtained by training $V(\theta)$ with the global and local cost functions respectively given by (31) and (32). Specifically, while we train with finite sampling, in the figures we show the exact cost-function values versus the number of iterations. Here, the top (bottom) axis corresponds to the number of iterations performed while training with C'_G (C'_L). For $n_B = 10$ and 15, Fig. 5 shows that we are able to train $V(\theta)$ for both cost functions.

For $n_B = 20$, the global cost function initially presents a plateau in which the optimizing algorithm is not able to determine a minimizing direction. However, as the number of shots per function evaluation increases, one can eventually minimize C_G' . Such result indicates the presence of a barren plateau where the gradient takes small values which can only be detected when the number of shots becomes sufficiently large. In this particular example, one is able to start training at around 140 iterations.

When $n_B > 20$ we are unable to train the global cost function, while always being able to train our proposed local cost function. Note that the number of iterations is different for C'_G and C'_L , as for the global cost function case we reach the maximum number of shots in fewer iterations. These results indicate that the global cost function of (31) exhibits a barren plateau where the gradient of the cost function vanishes exponentially with the number of qubits, and which arises even for constant depth ansatzes. We remark that in principle one can always find a minimizing direction when training C'_{G} , although this would require a number of shots that increases exponentially with n_B . Moreover, one can see in Fig. 5 that randomly initializing the parameters always leads to $C'_G \approx 1$ due to the narrow gorge phenomenon (see Prop. 1), i.e., where the probability of being near the global minimum vanishes exponentially with n_B .

On the other hand, Fig. 5 shows that the barren plateau is avoided when employing a local cost function since we can train C_L' for all considered values of n_B . Moreover, as seen in Fig. 5, C_L' can be trained with a small number of shots per cost-function evaluation (as small as 10 shots per evaluation). As previously mentioned, even if the ansatz employed in our heuristics is beyond the scope of our theorems, we still find cost-function-dependent barren plateaus, indicating that this phenomenon is more general than what we consider here.

III. Discussion

Rigorous scaling results are urgently needed for VQAs, which many researchers believe will provide the path to quantum advantage with near-term quantum computers. One of the few such results is the barren plateau theorem of Ref. [7], which holds for VQAs with deep, hardwareefficient ansatzes. In this work, we proved that the barren plateau phenomenon extends to VQAs with shallow ansatzes. The key to extending this phenomenon to shallow circuits was to consider the locality of the operator Othat defines the cost function C. Theorem 1 presented a universal upper bound on the variance of the gradient for global cost functions, i.e., when O is a global operator. Corollary 1 stated the asymptotic scaling of this upper bound for shallow ansatzes as being exponentially decaying in n, indicating a barren plateau. Conversely, Theorem 2 presented a universal lower bound on the variance of the gradient for local cost functions, i.e., when O is a sum of local operators. Corollary 2 notes that for

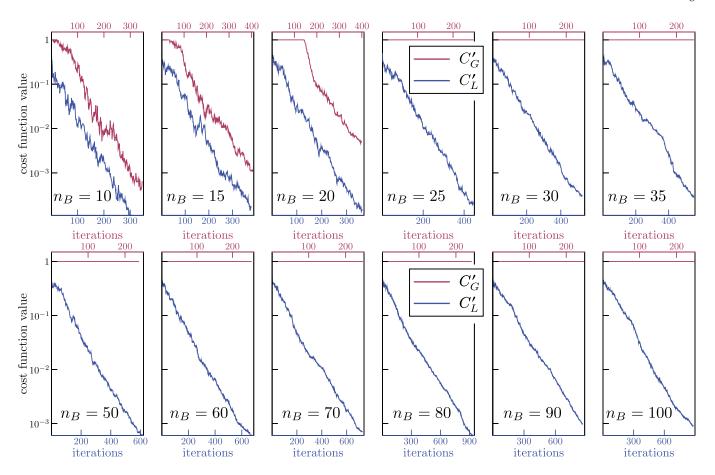


FIG. 5. Cost versus number of iterations for the quantum autoencoder problem defined by Eqs. (34)–(35). In all cases we employed two layers of the ansatz shown in Fig. 4, and we set $n_A=1$, while increasing $n_B=10,15,\ldots,100$. The top (bottom) axis corresponds to the global cost function C'_G of Eq. (31) (local cost function C'_L of (32)). As can be seen, C'_G can be trained up to $n_B=20$ qubits, while C'_L trained in all cases. These results indicate that global cost function presents a barren plateau even for a shallow depth ansatz, and this can be avoided by employing a local cost function.

shallow ansatzes this lower bound decays polynomially in n. Taken together, these two results show that barren plateaus are cost-function-dependent, and they establish a connection between locality and trainability.

We remark that our definition of a global operator (local operator) is one that is both non-local (local) and many body (few body). Therefore, the barren plateau phenomenon could be due to the many-bodiness of the operator rather than the non-locality of the operator; we leave the resolution of this question to future work. On the other hand, our Theorem 1 rules out the possibility that barren plateaus could be due to cardinality, i.e., the number of terms in O when decomposed as a sum of Pauli products [40]. Namely, from case (ii) of this theorem we can show that barren plateaus for O of arbitrary cardinality, and hence cardinality is not the key variable at work here.

We illustrated these ideas for two example VQAs. In Fig. 2, we considered a simple state-preparation example, which allowed us to delve deeper into the cost landscape and uncover another phenomenon that we called a narrow gorge, stated precisely in Prop. 1. In Fig. 5, we studied

the more important example of quantum autoencoders, which have generated significant interest in the quantum machine learning community. Our numerics showed the effects of barren plateaus: the global cost function introduced in [9] was untrainable for more than 20 qubits. To address this, we introduced a local cost function for quantum autoencoders, which we were able to minimize for system sizes of up to 100 qubits.

There are several directions in which our results could be generalized in future work. Naturally, we hope to extend the narrow gorge phenomenon in Prop. 1 to more general VQAs. In addition, we hope in the future to unify our theorems 1 and 2 into a single result that bounds the variance as a function of a parameter that quantifies the locality of O. This would further solidify the connection between locality and trainability. Moreover, our numerics suggest that our theorems (which are stated for exact 2-designs) could be extended in some form to approximate 2-designs [33].

Finally, we emphasize that our theorems are stated for a hardware-efficient ansatz $V(\theta)$. It remains an interesting open question as to whether other ansatzes, such

as the unitary-coupled cluster (UCC) ansatz in chemistry [41], exhibit similar scaling behavior as that stated in our theorems. The UCC ansatz is intended for use in the $\mathcal{O}(\operatorname{poly}(n))$ depth regime [30]. Therefore it is important to study the key mathematical features of an ansatz that might allow one to go from trainability for $\mathcal{O}(\log n)$ depth (which we guarantee here for local cost functions) to trainability for $\mathcal{O}(\operatorname{poly} n)$ depth.

IV. Methods

In this section, we provide a sketch of the proofs for our main theorems. We note that the proof of Theorem 2 comes before that of Theorem 1 since the latter builds on the former. More detailed proofs of our theorems are given in the Supplementary Information.

A. Computing averages over V

Here we introduce the main tools employed to compute quantities of the form $\langle \dots \rangle_V$. These tools are used throughout the proofs of our main results.

Let us first remark that if the blocks in $V(\theta)$ are independent, then any average over V can be computed by averaging over the individual blocks, i.e., $\langle \dots \rangle_V = \langle \dots \rangle_{W_{11},\dots,W_{kt},\dots} = \langle \dots \rangle_{V_L,W,V_R}$. For simplicity let us first consider the expectation value over a single block W in the ansatz. In principle $\langle \dots \rangle_W$ can be approximated by varying the parameters in W and sampling over the resulting $2^m \times 2^m$ unitaries. However, if W forms a t-design, this procedure can be simplified as it is known that sampling over its distribution yields the same properties as sampling random unitaries from the unitary group with respect to the unique normalized Haar measure.

Explicitly, the Haar measure is a uniquely defined left and right-invariant measure over the unitary group $d\mu(W)$, such that for any unitary matrix $A \in U(2^m)$ and for any function f(W) we have

$$\int_{U(2^m)} d\mu(W) f(W) = \int d\mu(W) f(AW)$$

$$= \int d\mu(W) f(WA),$$
(36)

where the integration domain is assumed to be $U(2^m)$ throughout this work. Then, a unitary t-design is defined as a finite set $\{W_y\}_{y\in Y}$ (of size |Y|) of unitaries W_y such that for every polynomial $P_{(t,t)}(W)$ of degree at most t in the matrix elements of W and at most t in those of W^{\dagger} [32] we have

$$\langle P_{(t,t)}(W) \rangle_w = \frac{1}{|Y|} \cdot \sum_{y \in Y} P_{(t,t)}(W_y)$$
$$= \int d\mu(W) P_{(t,t)}(W). \tag{37}$$

From the general form of C in Eq. (6) we can see the cost function is a polynomial of degree at most 2 in the matrix elements of each block W_{kl} in $V(\theta)$, and at most 2 in those of $(W_{kl})^{\dagger}$. Then, if a given block W forms a 2-design, one can employ the following elementwise formula of the Weingarten calculus [42] to explicitly evaluate averages over W up to the second moment:

$$\int d\mu(W) w_{ij} w_{i'j'}^* = \frac{\delta_{ii'} \delta_{jj'}}{2^m}$$

$$\int d\mu(W) w_{i_1j_1} w_{i_2j_2} w_{i'_1j'_1}^* w_{i'_2j'_2}^* = \frac{1}{2^{2m} - 1} \left(\Delta_1 - \frac{\Delta_2}{2^m} \right)$$
(38)

where w_{ij} are the matrix elements of W, and

$$\Delta_{1} = \delta_{i_{1}i'_{1}} \delta_{i_{2}i'_{2}} \delta_{j_{1}j'_{1}} \delta_{j_{2}j'_{2}} + \delta_{i_{1}i'_{2}} \delta_{i_{2}i'_{1}} \delta_{j_{1}j'_{2}} \delta_{j_{2}j'_{1}},
\Delta_{2} = \delta_{i_{1}i'_{1}} \delta_{i_{2}i'_{2}} \delta_{j_{1}j'_{1}} \delta_{j_{2}j'_{1}} + \delta_{i_{1}i'_{2}} \delta_{i_{2}i'_{1}} \delta_{j_{1}j'_{2}} \delta_{j_{2}j'_{1}}.$$
(39)

B. Sketch of the proof of the main theorems

Here we present a sketch of the proof of Theorem 1 and Theorem 2. We refer the reader to the Supplementary Information for a detailed version of the proofs.

As mentioned in the previous subsection, if each block in $V(\theta)$ forms a local 2-design, then we can explicitly calculate expectation values $\langle \dots \rangle_W$ via (38). Hence, to compute $\langle \Delta \Omega_{qp}^{p'q'} \rangle_{V_R}$, and $\langle \Delta \Psi_{pq}^{p'q'} \rangle_{V_L}$ in (14), one needs to algorithmically integrate over each block using the Weingarten calculus. In order to make such computation tractable, we employ the tensor network representation of quantum circuits.

For the sake of clarity, we recall that any two qubit gate can be expressed as $U = \sum_{ijkl} U_{ijkl} |ij\rangle\langle kl|$, where U_{ijkl} is a $2\times2\times2\times2$ tensor. Similarly, any block in the ansatz can be considered as a $2^{\frac{m}{2}}\times2^{\frac{m}{2}}\times2^{\frac{m}{2}}\times2^{\frac{m}{2}}$ tensor. As schematically shown in Fig. 6(a), one can use the circuit description of Ω^{i}_{qp} and Ψ_{pq} to derive the tensor network representation of terms such as $\text{Tr}[\Omega^{i}_{qp}\Omega^{j}_{q'p'}]$. Here, Ω^{i}_{qp} is obtained from (17) by simply replacing O with O_i .

In Fig. 6(b) we depict an example where we employ the tensor network representation of Ω^i_{qp} to compute the average of $\text{Tr}[\Omega^i_{qp}\Omega^j_{q'p'}]$, and $\text{Tr}[\Omega^i_{qp}]\text{Tr}[\Omega^j_{q'p'}]$. As expected, after each integration one obtains a sum of four new tensor networks according to Eq. (38).

1. Proof of Theorem 2

Let us first consider an m-local cost function C where O is given by (25), and where \widehat{O}_i acts non trivially in a given subsystem S_k of S. In particular, when \widehat{O}_i is of this form the proof is simplified, although the more general proof is presented in the Supplementary Information. If $S_k \not\subset S_{\mathcal{L}}$ we find $\Omega^i_{qp} \propto \mathbb{1}_w$, and hence

$$\operatorname{Tr}\left[\Omega_{\boldsymbol{q}\boldsymbol{p}}^{i}\Omega_{\boldsymbol{q}'\boldsymbol{p}'}^{j}\right] - \frac{\operatorname{Tr}\left[\Omega_{\boldsymbol{q}\boldsymbol{p}}^{i}\right]\operatorname{Tr}\left[\Omega_{\boldsymbol{q}'\boldsymbol{p}'}^{j}\right]}{2^{m}} = 0. \tag{40}$$

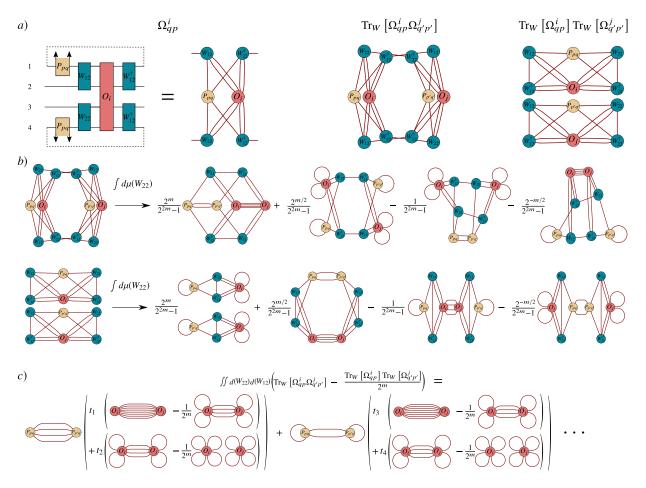


FIG. 6. Tensor-network representations of the terms relevant to $Var[\partial_{\nu}C]$. a) Representation of Ω_{qp}^{i} of Eq. (17) (left), where the superscript indicates that O is replaced by O_i . In this illustration, we show the case of n=2m qubits, and we denote $P_{pq} = |q\rangle\langle p|$. We also show the representation of $\text{Tr}[\Omega^i_{qp}\Omega^j_{q'p'}]$ (middle) and of $\text{Tr}[\Omega^i_{q'p'}]\text{Tr}[\Omega^j_{q'p'}]$ (right). (b) By means of the Weingarten calculus we can algorithmically integrate over each block in the ansatz. After each integration one obtains four new tensors according to Eq. (38). Here we show the tensor obtained after the integrations $\int d\mu(W) \text{Tr}[\Omega^i_{qp} \Omega^j_{q'p'}]$ and $\int d\mu(W) \text{Tr}[\Omega_{qp}^i] \text{Tr}[\Omega_{q'p'}^j]$, which are needed to compute $\langle \Delta \Omega_{qp}^{q'p'} \rangle_{V_R}$ as in Eq. (14). c) As shown in the Supplementary Information, the result of the integration is a sum of the form (47), where the deltas over p, q, p', and q' arise from the contractions between P_{pq} and $P_{p'q'}$.

The later implies that we only have to consider the operators \hat{O}_i which act on qubits inside of the forward lightcone \mathcal{L} of W.

Then, as shown in the Supplementary Information, we find

$$\left\langle \operatorname{Tr}[\Omega_{\boldsymbol{qp}}^{i}\Omega_{\boldsymbol{q'p'}}^{i}] - \frac{\operatorname{Tr}[\Omega_{\boldsymbol{qp}}^{i}]\operatorname{Tr}[\Omega_{\boldsymbol{q'p'}}^{i}]}{2^{m}} \right\rangle_{V_{R}} \propto \epsilon(\widehat{O}_{i}), \quad (41)$$

Here we remark that the proportionality factor contains terms of the form $\delta_{(\boldsymbol{p},\boldsymbol{q})_{S_{\overline{z}}^{+}}}\delta_{(\boldsymbol{p}',\boldsymbol{q}')_{S_{\overline{z}}^{+}}}\delta_{(\boldsymbol{p},\boldsymbol{q}')_{S_{\overline{z}}^{-}}}\delta_{(\boldsymbol{p}',\boldsymbol{q})_{S_{\overline{z}}^{-}}}$ (where $S_{\overline{w}}^+ \cup S_{\overline{w}}^- = S_{\overline{w}}$), which arises from the different tensor contractions of $P_{pq} = |q\rangle\langle p|$ in Fig. 6(c). It is then straightforward to show that

$$\sum_{\substack{\mathbf{p}\mathbf{q}\\\mathbf{p}'\mathbf{q}'}} \delta_{(\mathbf{p},\mathbf{q})_{S_{\overline{w}}^{+}}} \delta_{(\mathbf{p}',\mathbf{q}')_{S_{\overline{w}}^{+}}} \delta_{(\mathbf{p},\mathbf{q}')_{S_{\overline{w}}^{-}}} \delta_{(\mathbf{p}',\mathbf{q})_{S_{\overline{w}}^{-}}} \left\langle \Delta \Psi_{\mathbf{p}\mathbf{q}}^{\mathbf{p}'\mathbf{q}'} \right\rangle_{V_{L}}$$

$$= \left\langle D_{\mathrm{HS}} \left(\tilde{\rho}^{-}, \mathrm{Tr}_{w} [\tilde{\rho}^{-}] \otimes \frac{1}{2^{m}} \right) \right\rangle_{V_{L}}, \tag{42}$$

where we define $\tilde{\rho}^-$ as the reduced states of $\tilde{\rho} = V_L \rho V_L^{\intercal}$ in the Hilbert spaces associated with subsystems $S_w \cup S_{\overline{w}}^-$. By employing properties of the Hilbert-Schmidt dis-

tance one can show (see Supplementary Information)

$$D_{\mathrm{HS}}\left(\tilde{\rho}^{-}, \mathrm{Tr}_{w}[\tilde{\rho}^{-}] \otimes \frac{1}{2^{m}}\right) \geqslant \frac{D_{\mathrm{HS}}\left(\tilde{\rho}_{w}, \frac{1}{2^{m}}\right)}{2^{m(L-l+2)/2}}, \quad (43)$$

where $\tilde{\rho}_w = \text{Tr}_{S_{-}}[\tilde{\rho}^-]$. We can then leverage the tensor network representation of quantum circuits to algorithmically integrate over each block in V_L and compute $\langle D_{\mathrm{HS}}\left(\widetilde{\rho}_w, \frac{1}{2^m}\right)\rangle_{V_L}$. One finds

$$\left\langle D_{\mathrm{HS}}\left(\tilde{\rho}_{w}, \frac{1}{2^{m}}\right)\right\rangle_{V_{L}} = \sum_{\substack{(k, k') \in k_{\mathcal{L}_{B}} \\ k' \geqslant k}} t_{k, k'} \epsilon(\rho_{k, k'}) \qquad (44)$$

with $t_{k,k'} \geqslant \frac{2^{ml}}{(2^m+1)^{2l}} \ \forall k,k'$, and $\epsilon(\rho_{k,k'})$ defined in Theorem 2. Combining these results leads to Theorem 2. Moreover, as detailed in the Supplementary information, Theorem 2 is also valid when O is of the form (25).

2. Proof of Theorem 1

Let us now provide a sketch of the proof of Theorem 1, case (i). Here we denote for simplicity $\widehat{O}_k := \widehat{O}_{1k}$. We leave the proof of case (ii) for the Supplementary Information. In this case there are now operators O_i which act outside of the forward light-cone \mathcal{L} of W. Hence, it is convenient to include in V_R not only all the gates in \mathcal{L} but also all the blocks in the final layer of $V(\boldsymbol{\theta})$ (i.e., all blocks W_{kL} , with $k = 1, ... \xi$). We can define $S_{\overline{L}}$ as the compliment of $S_{\mathcal{L}}$, i.e., as the subsystem of all qubits which are not in \mathcal{L} (with associated Hilbert-space $\mathcal{H}_{\overline{\mathcal{L}}}$). Then, we have $V_R = V_{\mathcal{L}} \otimes V_{\overline{\mathcal{L}}}$ and $|\mathbf{q}\rangle\langle\mathbf{p}| = |\mathbf{q}\rangle\langle\mathbf{p}|_{\mathcal{L}} \otimes |\mathbf{q}\rangle\langle\mathbf{p}|_{\overline{\mathcal{L}}}, \text{ where we define } V_{\overline{\mathcal{L}}} := \bigotimes_{k \in k_{\overline{\mathcal{L}}}} W_{kL}, |\mathbf{q}\rangle\langle\mathbf{p}|_{\mathcal{L}} := \bigotimes_{k \in k_{\mathcal{L}}} |\mathbf{q}\rangle\langle\mathbf{p}|_{k}, \text{ and } |\mathbf{q}\rangle\langle\mathbf{p}|_{\overline{\mathcal{L}}} := \bigotimes_{k' \in k_{\overline{\mathcal{L}}}} |\mathbf{q}\rangle\langle\mathbf{p}|_{k'}. \text{ Here, we define } k_{\mathcal{L}} := \{k : S_k \subseteq S_{\mathcal{L}}\}$ and $k_{\overline{L}} := \{k : S_k \subseteq S_{\overline{L}}\}$, which are the set of indices whose associated qubits are inside and outside \mathcal{L} , respectively. We also write $O = c_0 \mathbb{1} + c_1 \hat{O}_{\mathcal{L}} \otimes \hat{O}_{\overline{\mathcal{L}}}$, where we define $\hat{O}_{\mathcal{L}} := \bigotimes_{k \in k_{\mathcal{L}}} \hat{O}_k$ and $\hat{O}_{\overline{\mathcal{L}}} := \bigotimes_{k' \in k_{\overline{\mathcal{L}}}} \hat{O}_{k'}$.

Using the fact that the blocks in $V(\boldsymbol{\theta})$ are independently and $\hat{O}_{\mathcal{L}} := \bigotimes_{k' \in k_{\overline{\mathcal{L}}}} \hat{O}_{k'}$.

Using the fact that the blocks in $V(\boldsymbol{\theta})$ are independent we can now compute $\langle \Delta \Omega_{\boldsymbol{qp}}^{\boldsymbol{q'p'}} \rangle_{V_R} = \langle \Delta \Omega_{\boldsymbol{qp}}^{\boldsymbol{q'p'}} \rangle_{V_{\overline{L}},V_{\mathcal{L}}}$. Then, from the definition of $\Omega_{\boldsymbol{pq}}$ in Eq. (17) and the fact that one can always express

$$\left\langle \Delta \Omega_{\boldsymbol{q}\boldsymbol{p}}^{\boldsymbol{q'}\boldsymbol{p'}} \right\rangle_{V_R} = \left\langle \operatorname{Tr}[\Omega_{\boldsymbol{q}\boldsymbol{p}}^{\mathcal{L}}\Omega_{\boldsymbol{q'}\boldsymbol{p'}}^{\mathcal{L}}] - \frac{\operatorname{Tr}[\Omega_{\boldsymbol{q}\boldsymbol{p}}^{\mathcal{L}}]\operatorname{Tr}[\Omega_{\boldsymbol{q'}\boldsymbol{p'}}^{\mathcal{L}}]}{2^m} \right\rangle_{V_{\mathcal{L}}} \times \left(\prod_{k \in k_{\overline{\mathcal{L}}}} \left\langle \Omega_k \right\rangle_{W_{kL}} \right) , \tag{45}$$

with

$$\Omega_{\boldsymbol{q}\boldsymbol{p}}^{\mathcal{L}} = \operatorname{Tr}_{\mathcal{L}\cap\overline{w}}\left[(|\boldsymbol{p}\rangle\langle\boldsymbol{q}|\otimes\mathbb{1}_{w})V_{\mathcal{L}}O^{\mathcal{L}}V_{\mathcal{L}}\right]
\Omega_{k} = \operatorname{Tr}\left[|\boldsymbol{p}\rangle\langle\boldsymbol{q}|_{k}W_{kL}^{\dagger}\widehat{O}_{k}W_{kL}\right]\operatorname{Tr}\left[|\boldsymbol{p}'\rangle\langle\boldsymbol{q}'|_{k}W_{kL}^{\dagger}\widehat{O}_{k}W_{kL}\right]$$

and where $\operatorname{Tr}_{\mathcal{L}\cap\overline{w}}$ indicates the partial trace over the Hilbert-space associated with the qubits in $S_{\mathcal{L}} \cap S_{\overline{w}}$. As detailed in the Supplementary Information we can use Eq. (38) to show that

$$\langle \Omega_k \rangle_{W_{kL}} \leqslant \frac{r_k^2 \left(\delta_{(\boldsymbol{p},\boldsymbol{q})_{S_k}} \delta_{(\boldsymbol{p'},\boldsymbol{q'})_{S_k}} + \delta_{(\boldsymbol{p},\boldsymbol{q'})_{S_k}} \delta_{(\boldsymbol{p'},\boldsymbol{q})_{S_k}} \right)}{2^{2m} - 1} . \tag{46}$$

On the other hand, as shown in the Supplementary Information (and as schematically depicted in Fig. 6(c)), when computing the expectation value $\langle \dots \rangle_{V_{\mathcal{L}}}$ in (45), one obtains

$$\left\langle \operatorname{Tr}[\Omega_{\boldsymbol{qp}}^{\mathcal{L}}\Omega_{\boldsymbol{q'p'}}^{\mathcal{L}}] - \frac{\operatorname{Tr}[\Omega_{\boldsymbol{qp}}^{\mathcal{L}}]\operatorname{Tr}[\Omega_{\boldsymbol{q'p'}}^{\mathcal{L}}]}{2^{m}} \right\rangle_{V_{\mathcal{L}}} = \sum_{\tau} t_{\tau}^{ij} \Delta O_{\tau}^{\mathcal{L}} \delta_{\tau},$$

$$(47)$$

where we defined $\delta_{\tau} = \delta_{(\boldsymbol{p},\boldsymbol{q})_{S_{\overline{\tau}}}} \delta_{(\boldsymbol{p}',\boldsymbol{q}')_{S_{\overline{\tau}}}} \delta_{(\boldsymbol{p},\boldsymbol{q}')_{S_{\tau}}} \delta_{(\boldsymbol{p}',\boldsymbol{q})_{S_{\tau}}},$ $t_{\tau} \in \mathbb{R}, \ S_{\tau} \cup S_{\overline{\tau}} = S_{\mathcal{L}} \cap S_{\overline{w}} \ (\text{with} \ S_{\tau} \neq \emptyset), \ \text{and}$

$$\Delta O_{\tau}^{\mathcal{L}} = \operatorname{Tr}_{x_{\tau}y_{\tau}} \left[\operatorname{Tr}_{z_{\tau}} \left[O_{i} \right] \operatorname{Tr}_{z_{\tau}} \left[O_{j} \right] \right] - \frac{\operatorname{Tr}_{x_{\tau}} \left[\operatorname{Tr}_{y_{\tau}z_{\tau}} \left[O_{i} \right] \operatorname{Tr}_{y_{\tau}z_{\tau}} \left[O_{j} \right] \right]}{2^{m}} .$$

$$(48)$$

Here we use the notation $\operatorname{Tr}_{x_{\tau}}$ to indicate the trace over the Hilbert space associated with subsystem $S_{x_{\tau}}$, such that $S_{x_{\tau}} \cup S_{y_{\tau}} \cup S_{z_{\tau}} = S_{\mathcal{L}}$. As shown in the Supplementary Information, combining the deltas in Eqs. (46), and (47) with $\left\langle \Delta \Psi_{pq}^{p'q'} \right\rangle_{V_L}$ leads to Hilbert-Schmidt distances between two quantum states as in (42). One can then use the following bounds $D_{\mathrm{HS}}\left(\rho_1,\rho_2\right) \leqslant 2$, $\Delta O_{\tau}^{\mathcal{L}} \leqslant \prod_{k \in k_{\mathcal{L}}} r_k^2$, and $\sum_{\tau} t_{\tau} \leqslant 2$, along with some additional simple algebra explained in the Supplementary Information to obtain the upper bound in Theorem 1.

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Supplementary Information for "Cost-Function-Dependent Barren Plateaus in Shallow Quantum Neural Networks"

In this Supplementary Information, we present detailed proofs of the propositions, theorems, and corollaries presented in the manuscript "Cost-Function-Dependent Barren Plateaus in Shallow Quantum Neural Networks". In Supplementary Note 1 we first introduce several lemmas which will be useful in the derivation of our main results. Then, in Supplementary Note 2, and Supplementary Note 3 we respectively provide proofs for Propositions 1 and 2 of the main text. We then derive the general equations for the variance of the cost function partial derivative in Supplementary Note 4. In Supplementary Note 5 we explicitly evaluate the variance of the cost function derivative for the special case when $V(\theta)$ is given by a single layer of the Alternating Layered Ansatz.

In Supplementary Note 6, and Supplementary Note 7, we provide our proofs to Theorem 2 and Theorem 1, respectively. Where we remark that the proof of Theorem 2 comes before that of Theorem 1 since the latter builds on the former. Then, in Supplementary Note 8, we prove Corollaries 1, and 2. In Supplementary Note 9, we demonstrate that the local cost function for the quantum autoencoder is faithful.

Supplementary Note 1: Preliminaries

In this section, we present properties that allow for analytic calculation of integrals of polynomial functions over the unitary group with respect to the unique normalized Haar measure. For more details on this topic, we refer the reader to Ref. [42]. In addition, to make the Supplementary Information more self-contained, we reiterate here the definition of a t-design. A unitary t-design is defined as a finite set $\{W_y\}_{y\in Y}$ (of size |Y|) of unitaries W_y on a d-dimensional Hilbert space such that for every polynomial $P_{(t,t)}(W)$ of degree at most t in the matrix elements of W and at most t in those of W^{\dagger} [32], we have

$$\frac{1}{|Y|} \cdot \sum_{y \in Y} P_{(t,t)}(W_y) = \int_{U(d)} d\mu(W) P_{(t,t)}(W), \qquad (49)$$

where in the right-hand side U(d) denotes the unitary group of degree d. Equation (49) implies that averaging $P_{(t,t)}(W)$ over the t-design is indistinguishable from integrating over U(d) with respect to the Haar distribution. Given $W \in U(d)$ the following expressions are valid for the first two moments

$$\int_{U(d)} d\mu(W) w_{i,j} w_{\mathbf{p},\mathbf{k}}^* = \frac{\delta_{i,\mathbf{p}} \delta_{j,\mathbf{k}}}{d}, \qquad (50)$$

$$\int_{U(d)} d\mu(W) w_{i_1,j_1} w_{i_2,j_2} w_{i'_1,j'_1}^* w_{i'_2,j'_2}^* = \frac{1}{d^2 - 1} \left(\delta_{i_1,i'_1} \delta_{i_2,i'_2} \delta_{j_1,j'_1} \delta_{j_2,j'_2} + \delta_{i_1,i'_2} \delta_{i_2,i'_1} \delta_{j_1,j'_2} \delta_{j_2,j'_1} \right)$$

$$- \frac{1}{d(d^2 - 1)} \left(\delta_{i_1,i'_1} \delta_{i_2,i'_2} \delta_{j_1,j'_2} \delta_{j_2,j'_1} + \delta_{i_1,i'_2} \delta_{i_2,i'_1} \delta_{j_1,j'_1} \delta_{j_2,j'_2} \right). \qquad (51)$$

All throughout this section the integration domain will be implied to be U(d), and unless otherwise specified we consider W to be an operator acting on a Hilbert space \mathcal{H}_w of dimension d. When $d=2^m$, as occurs for a Hilbert space of m qubit, we adopt the symbol $\mathbf{i}=(i_1,\ldots i_m)$ to denote a bitstring of length m such that $i_1,i_2,\ldots,i_m\in\{0,1\}$. Moreover, given two bitstrings \mathbf{i} and \mathbf{j} we define their concatenation as $\mathbf{i}\cdot\mathbf{j}=(i_1,\ldots i_n,j_1,\ldots j_n)$.

Operators in the computational basis of m qubits can be written as

$$W = \sum_{i,j} w_{i,j} |i\rangle \langle j|, \quad W^{\dagger} = \sum_{i',j'} w_{i',j'}^* |j'\rangle \langle i'|, \quad A = \sum_{k,l} a_{k,l} |k\rangle \langle l|, \quad B = \sum_{q,p} b_{q,p} |q\rangle \langle p|.$$

These expressions lead to the following lemmas.

Lemma 1. Let $\{W_y\}_{y\in Y}\subset U(d)$ form a unitary t-design with $t\geq 1$, and let $A,B:\mathcal{H}_w\to\mathcal{H}_w$ be arbitrary linear operators. Then

$$\frac{1}{|Y|} \sum_{y \in Y} \operatorname{Tr} \left[W_y A W_y^{\dagger} B \right] = \int d\mu(W) \operatorname{Tr} \left[W A W^{\dagger} B \right] = \frac{\operatorname{Tr} \left[A \right] \operatorname{Tr} \left[B \right]}{d}. \tag{52}$$

Proof. The first equality follows from the definition of a t-design given above. Note that $\text{Tr}\left[WAW^{\dagger}B\right]$ can be written as

$$\text{Tr}\left[WAW^{\dagger}B\right] = \sum_{\boldsymbol{i}_{1},\boldsymbol{j}_{1},\boldsymbol{i}_{1}',j_{1}'} a_{\boldsymbol{j}_{1},\boldsymbol{j}_{1}'} b_{\boldsymbol{i}_{1}',\boldsymbol{i}_{1}} w_{\boldsymbol{i}_{1},\boldsymbol{j}_{1}} w_{\boldsymbol{i}_{1}',\boldsymbol{j}_{1}'}^{*}.$$

Then, from (50), we have

$$\int d\mu(W) \mathrm{Tr} \left[WAW^{\dagger}B \right] = \frac{1}{d} \sum_{\boldsymbol{i_1,j_1}} a_{\boldsymbol{j_1,j_1}} b_{\boldsymbol{i_1,i_1}} = \frac{\mathrm{Tr} \left[A \right] \mathrm{Tr} \left[B \right]}{d} \,.$$

Lemma 2. Let $\{W_y\}_{y\in Y}\subset U(d)$ form a unitary t-design with $t\geq 2$ and let $A,B,C,D:\mathcal{H}_w\to\mathcal{H}_w$ be arbitrary linear operators. Then

$$\frac{1}{|Y|} \sum_{y \in Y} \operatorname{Tr}[W_y A W_y^{\dagger} B W_y C W_y^{\dagger} D] = \int d\mu(W) \operatorname{Tr}[W A W^{\dagger} B W C W^{\dagger} F]$$

$$= \frac{1}{d^2 - 1} \left(\operatorname{Tr}[A] \operatorname{Tr}[C] \operatorname{Tr}[B D] + \operatorname{Tr}[A C] \operatorname{Tr}[B] \operatorname{Tr}[D] \right)$$

$$- \frac{1}{d(d^2 - 1)} \left(\operatorname{Tr}[A C] \operatorname{Tr}[B D] + \operatorname{Tr}[A] \operatorname{Tr}[B] \operatorname{Tr}[C] \operatorname{Tr}[D] \right) .$$
(53)

Proof. The first equality follows from that fact that $\text{Tr}[W_yAW_y^{\dagger}BW_yCW_y^{\dagger}F] \in P_{(2,2)}(V_y)$. By writting

$$\operatorname{Tr}[WAW^{\dagger}BWCW^{\dagger}D] = \sum_{\substack{\boldsymbol{i}_{1},\boldsymbol{j}_{1},\boldsymbol{i}_{1}',\boldsymbol{j}_{1}'\\\boldsymbol{i}_{2},\boldsymbol{j}_{2},\boldsymbol{i}_{2}',\boldsymbol{j}_{2}'}} a_{\boldsymbol{j}_{1},\boldsymbol{j}_{1}'}b_{\boldsymbol{i}_{1}',\boldsymbol{i}_{2}}c_{\boldsymbol{j}_{2},\boldsymbol{j}_{2}'}d_{\boldsymbol{i}_{2}',\boldsymbol{i}_{1}}w_{\boldsymbol{i}_{1},\boldsymbol{j}_{1}}w_{\boldsymbol{i}_{2},\boldsymbol{j}_{2}}w_{\boldsymbol{i}_{1}',\boldsymbol{j}_{1}'}^{*}w_{\boldsymbol{i}_{2}',\boldsymbol{j}_{2}'}^{*},$$

we can use (51) to obtain

$$\int d\mu(W) \text{Tr}[WAW^{\dagger}BWCW^{\dagger}D] = \frac{1}{d^{2}-1} \sum_{i_{1},j_{1},i_{2},j_{2}} \left(a_{j_{1},j_{1}} b_{i_{1},i_{2}} c_{j_{2},j_{2}} d_{i_{2},i_{1}} + a_{j_{1},j_{2}} b_{i_{2},i_{2}} c_{j_{2},j_{1}} d_{i_{1},i_{1}} \right)
- \frac{1}{d(d^{2}-1)} \sum_{i_{1},j_{1},i_{2},j_{2}} \left(a_{j_{1},j_{2}} b_{i_{1},i_{2}} c_{j_{2},j_{1}} d_{i_{2},i_{1}} + a_{j_{1},j_{1}} b_{i_{2},i_{2}} c_{j_{2},j_{2}} d_{i_{1},i_{1}} \right)
= \frac{1}{d^{2}-1} \left(\text{Tr}[A] \text{Tr}[C] \text{Tr}[BD] + \text{Tr}[AC] \text{Tr}[B] \text{Tr}[D] \right)
- \frac{1}{d(d^{2}-1)} \left(\text{Tr}[AC] \text{Tr}[BD] + \text{Tr}[A] \text{Tr}[B] \text{Tr}[C] \text{Tr}[D] \right) .$$
(54)

Lemma 3. Let $\{W_y\}_{y\in Y}\subset U(d)$ form a unitary t-design with $t\geq 2$ and let $A,B,C,D:\mathcal{H}_w\to\mathcal{H}_w$ be arbitrary linear operators. Then

$$\begin{split} \frac{1}{|Y|} \sum_{y \in Y} \mathrm{Tr}[W_y A W_y^\dagger B] \mathrm{Tr}[W_y C W_y^\dagger D] &= \int d\mu(W) \mathrm{Tr}[W A W^\dagger B] \mathrm{Tr}[W C W^\dagger D] \\ &= \frac{1}{d^2 - 1} \left(\mathrm{Tr}[A] \mathrm{Tr}[B] \mathrm{Tr}[C] \mathrm{Tr}[D] + \mathrm{Tr}[A C] \mathrm{Tr}[B D] \right) \\ &- \frac{1}{d(d^2 - 1)} \left(\mathrm{Tr}[A C] \mathrm{Tr}[B] \mathrm{Tr}[D] + \mathrm{Tr}[A] \mathrm{Tr}[C] \mathrm{Tr}[B D] \right) \,. \end{split}$$

Proof. The first equality follows from a reasoning similar to the one used in Lemma 2. By expressing

$$\operatorname{Tr}\left[WAW^{\dagger}B\right]\operatorname{Tr}\left[WCW^{\dagger}D\right] = \sum_{\boldsymbol{\alpha},\boldsymbol{\beta}}\operatorname{Tr}\left[WAW^{\dagger}B|\boldsymbol{\alpha}\rangle\langle\boldsymbol{\beta}|WCW^{\dagger}D|\boldsymbol{\beta}\rangle\langle\boldsymbol{\alpha}|\right]\,,$$

we can employ (53) to obtain

$$\begin{split} \int d\mu(W) \mathrm{Tr}[WAW^{\dagger}B] \mathrm{Tr}[WCW^{\dagger}D] &= \sum_{\pmb{\alpha},\pmb{\beta}} \int d\mu(W) \mathrm{Tr}\left[WAW^{\dagger}B|\pmb{\alpha}\rangle\langle\pmb{\beta}|WCW^{\dagger}D|\pmb{\beta}\rangle\langle\pmb{\alpha}|\right] \\ &= \frac{1}{d^2-1} \sum_{\pmb{\alpha},\pmb{\beta}} \left(\mathrm{Tr}[A] \mathrm{Tr}[C] \langle \pmb{\alpha}|B|\pmb{\alpha}\rangle\langle\pmb{\beta}|D|\pmb{\beta}\rangle + \mathrm{Tr}[AC] \langle \pmb{\beta}|B|\pmb{\alpha}\rangle\langle\pmb{\alpha}|D|\pmb{\beta}\rangle \right) \\ &- \frac{1}{d(d^2-1)} \sum_{\pmb{\alpha},\pmb{\beta}} \left(\mathrm{Tr}[AC] \langle \pmb{\alpha}|B|\pmb{\alpha}\rangle\langle\pmb{\beta}|D|\pmb{\beta}\rangle + \mathrm{Tr}[A] \mathrm{Tr}[C] \langle \pmb{\beta}|B|\pmb{\alpha}\rangle\langle\pmb{\alpha}|D|\pmb{\beta}\rangle \right) \\ &= \frac{1}{d^2-1} \left(\mathrm{Tr}[A] \mathrm{Tr}[B] \mathrm{Tr}[C] \mathrm{Tr}[D] + \mathrm{Tr}[AC] \mathrm{Tr}[BD] \right) \\ &- \frac{1}{d(d^2-1)} \left(\mathrm{Tr}[AC] \mathrm{Tr}[B] \mathrm{Tr}[D] + \mathrm{Tr}[A] \mathrm{Tr}[C] \mathrm{Tr}[BD] \right) \; . \end{split}$$

Lemma 4. Let $\mathcal{H} = \mathcal{H}_{\overline{w}} \otimes \mathcal{H}_w$ be a bipartite Hilbert space of dimension $d = d_{\overline{w}}d_w$, and let $\{W_y\}_{y \in Y}$ be a unitary t-design with $t \geq 1$ such that $W_y \in U(d_w)$ for all $y \in Y$. Then for arbitrary linear operators $A, B : \mathcal{H} \to \mathcal{H}$, it follows

$$\int d\mu(W) (\mathbb{1}_{\overline{w}} \otimes W) A (\mathbb{1}_{\overline{w}} \otimes W^{\dagger}) B = \frac{\operatorname{Tr}_{w} [A] \otimes \mathbb{1}_{w}}{d_{w}} B, \qquad (55)$$

and

$$\int d\mu(W) \operatorname{Tr}\left[\left(\mathbb{1}_{\overline{w}} \otimes W\right) A\left(\mathbb{1}_{\overline{w}} \otimes W^{\dagger}\right) B\right] = \frac{1}{d_w} \operatorname{Tr}\left[\operatorname{Tr}_w\left[A\right] \operatorname{Tr}_w\left[B\right]\right]. \tag{56}$$

Here we use the notation $\mathbb{1}_w$ to indicate the identity operator on subsystem \mathcal{H}_w , and we employ Tr_w to indicate the partial trace over \mathcal{H}_w .

Proof. First, note that

$$(\mathbb{1}_{\overline{w}} \otimes W) A(\mathbb{1}_{\overline{w}} \otimes W^{\dagger}) B = \sum_{\boldsymbol{i}, \boldsymbol{i}, \boldsymbol{i}', \boldsymbol{j}'} w_{\boldsymbol{i}', \boldsymbol{j}'} (\mathbb{1}_{\overline{w}} \otimes |\boldsymbol{i}\rangle\langle \boldsymbol{j}|) A(\mathbb{1}_{\overline{w}} \otimes |\boldsymbol{j}'\rangle\langle \boldsymbol{i}'|) B,$$

by using (50) we have

$$\int d\mu(W)(\mathbb{1}_{\overline{w}} \otimes W)A(\mathbb{1}_{\overline{w}} \otimes W^{\dagger})B = \sum_{i,j,i',j'} \int d\mu(W)w_{i,j}w_{i',j'}^{*}(\mathbb{1}_{\overline{w}} \otimes |i\rangle\langle j|)A(\mathbb{1}_{\overline{w}} \otimes |j'\rangle\langle i'|)B$$

$$= \frac{1}{d_{w}} \sum_{i,j} (\mathbb{1}_{\overline{w}} \otimes |i\rangle\langle j|)A(\mathbb{1}_{\overline{w}} \otimes |j\rangle\langle i|)B$$

$$= \frac{1}{d_{w}} (\operatorname{Tr}_{w} [A] \otimes \mathbb{1}_{w}) B.$$

Finally we can also obtain

$$\int d\mu(W) \operatorname{Tr} \left[(\mathbb{1}_{\overline{w}} \otimes W) A (\mathbb{1}_{\overline{w}} \otimes W^{\dagger}) B \right] = \frac{1}{d_w} \operatorname{Tr} \left[\operatorname{Tr}_w \left[A \right] \operatorname{Tr}_w \left[B \right] \right].$$

Lemma 5. If $\mathcal{H} = \mathcal{H}_{\overline{w}} \otimes \mathcal{H}_w$ is a bipartite Hilbert space of dimension $d = d_{\overline{w}} d_w$, and if $A, B : \mathcal{H} \to \mathcal{H}$ are arbitrary linear operators, then for any linear operator $W: \mathcal{H}_w \to \mathcal{H}_w$ we have

$$\operatorname{Tr}\left[\left(\mathbb{1}_{\overline{w}}\otimes W\right)A(\mathbb{1}_{\overline{w}}\otimes W^{\dagger})B\right] = \sum_{\boldsymbol{p},\boldsymbol{q}}\operatorname{Tr}\left[WA_{\boldsymbol{q}\boldsymbol{p}}W^{\dagger}B_{\boldsymbol{p}\boldsymbol{q}}\right],\tag{57}$$

where the summation runs over all bitstrings of length $d_{\overline{w}}$, and where

$$A_{qp} = \operatorname{Tr}_{\overline{w}} \left[(|p\rangle \langle p|q \otimes \mathbb{1}_w) A \right], \quad B_{pq} = \operatorname{Tr}_{\overline{w}} \left[(|q\rangle \langle p| \otimes \mathbb{1}_w) B \right]. \tag{58}$$

Proof. By expanding the operators in the computational basis

$$\mathbb{1}_{\overline{w}} \otimes W = \sum_{\boldsymbol{p}, \boldsymbol{i}, \boldsymbol{j}} w_{\boldsymbol{i}, \boldsymbol{j}} |\boldsymbol{p}\rangle \langle \boldsymbol{p}| \otimes |\boldsymbol{i}\rangle \langle \boldsymbol{j}|, \qquad \mathbb{1}_{\overline{w}} \otimes W^{\dagger} = \sum_{\boldsymbol{q}, \boldsymbol{i}', \boldsymbol{j}'} w_{\boldsymbol{i}', \boldsymbol{j}'}^* |\boldsymbol{q}\rangle \langle \boldsymbol{q}| \otimes |\boldsymbol{j}'\rangle \langle \boldsymbol{i}'|, \qquad (59)$$

$$A = \sum_{\substack{\mathbf{k}_1, \mathbf{k}_2 \\ l_1, l_2}} a_{\mathbf{k}_1 \cdot \mathbf{k}_2, \mathbf{l}_1 \cdot l_2} |\mathbf{k}_1\rangle \langle \mathbf{l}_1| \otimes |\mathbf{k}_2\rangle \langle \mathbf{l}_2|, \quad B = \sum_{\substack{\mathbf{p}_1, \mathbf{p}_2 \\ \mathbf{q}_1, \mathbf{q}_2}} b_{\mathbf{p}_1 \cdot \mathbf{p}_2, \mathbf{q}_1 \cdot \mathbf{q}_2} |\mathbf{p}_1\rangle \langle \mathbf{q}_1| \otimes |\mathbf{p}_2\rangle \langle \mathbf{q}_2|, \quad (60)$$

we have

$$\operatorname{Tr}\left[\left(\mathbb{1}_{\overline{w}} \otimes W\right) A(\mathbb{1}_{\overline{w}} \otimes W^{\dagger}) B\right] = \sum_{\substack{i,j,i',j'\\ p,q}} w_{i,j} a_{p\cdot j,q\cdot i'} w_{i',j'} b_{q\cdot j',p\cdot i} = \sum_{p,q} \operatorname{Tr}\left[W A_{qp} W^{\dagger} B_{pq}\right]. \tag{61}$$

Lemma 6. Let $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \mathcal{H}_3 \otimes \mathcal{H}_4$ be a Hilbert space of dimension $d = d \cdot d \cdot d \cdot d = d^4$, and let $W : \mathcal{H}_1 \otimes \mathcal{H}_2 \to \mathcal{H}_3 \otimes \mathcal{H}_4$ $\mathcal{H}_1 \otimes \mathcal{H}_2$ be a t-design with $t \geq 2$. For arbitrary linear operators $A, A' : \mathcal{H} \to \mathcal{H}$ we define

$$\Omega_1 = (W \otimes \mathbb{1}_3 \otimes \mathbb{1}_4) A(W^{\dagger} \otimes \mathbb{1}_3 \otimes \mathbb{1}_4) (|\mathbf{p}\rangle\langle \mathbf{q}| \otimes \mathbb{1}_2 \otimes \mathbb{1}_3 \otimes \mathbb{1}_4), \quad \Omega_2 = (W \otimes \mathbb{1}_3 \otimes \mathbb{1}_4) A(W^{\dagger} \otimes \mathbb{1}_3 \otimes \mathbb{1}_4), \quad (62)$$

$$\Omega_1' = (W \otimes \mathbb{1}_3 \otimes \mathbb{1}_4) A'(W^{\dagger} \otimes \mathbb{1}_3 \otimes \mathbb{1}_4) (|\mathbf{p}'\rangle\langle \mathbf{q}'| \otimes \mathbb{1}_2 \otimes \mathbb{1}_3 \otimes \mathbb{1}_4), \quad \Omega_2' = (W \otimes \mathbb{1}_3 \otimes \mathbb{1}_4) A'(W^{\dagger} \otimes \mathbb{1}_3 \otimes \mathbb{1}_4), \quad (63)$$

where p, q, p', and q' are bitstrings of length d.

Let us first consider the quantity

$$\Delta\Omega_{jkl}^{(1)} = \operatorname{Tr}_{kl} \left[\operatorname{Tr}_{1j}[\Omega_1] \operatorname{Tr}_{1j}[\Omega'_1] \right] - \frac{\operatorname{Tr}_{l} \left[\operatorname{Tr}_{1jk}[\Omega_1]_{1jk} \operatorname{Tr}[\Omega'_1] \right]}{d_k}, \tag{64}$$

where Tr_j indicates the partial trace over \mathcal{H}_j , $\operatorname{Tr}_{jk} := \operatorname{Tr}_j \operatorname{Tr}_k$, and where we defined $\mathcal{H}_j \otimes \mathcal{H}_k \otimes \mathcal{H}_l = \mathcal{H}_2 \otimes \mathcal{H}_3 \otimes \mathcal{H}_4$. Moreover, one can always choose $\mathcal{H}_j = \mathcal{H}_0 := \{0\}$, in which case for any operator O we define the partial trace over \mathcal{H}_0 as $\operatorname{Tr}_0[O] := O$, and $\operatorname{Tr}_{j0}[O] := \operatorname{Tr}_j[O]$. Then, for $\mathcal{H}_k \in \{\mathcal{H}_2, \mathcal{H}_3, \mathcal{H}_2 \otimes \mathcal{H}_3, \mathcal{H}_3 \otimes \mathcal{H}_4\}$, the following equality always holds

$$\int d\mu(W) \Delta\Omega_{jkl}^{(1)} = \frac{t_1^{(1)} \delta_{pq'} \delta_{p'q}}{d^4 - 1} \left(\operatorname{Tr}_{123x} [\operatorname{Tr}_y[A] \operatorname{Tr}_y[A']] - \frac{\operatorname{Tr}_{3x} [\operatorname{Tr}_{12y}[A] \operatorname{Tr}_{12y}[A']]}{d^2} \right)
+ \frac{t_2^{(1)} \delta_{pq} \delta_{p'q'}}{d^4 - 1} \left(\operatorname{Tr}_{3x} [\operatorname{Tr}_{12y}[A] \operatorname{Tr}_{12y}[A']] - \frac{\operatorname{Tr}_x [\operatorname{Tr}_{123y}[A] \operatorname{Tr}_{123y}[A']]}{d'} \right)
- \frac{t_3^{(1)} \delta_{pq'} \delta_{p'q}}{d^4 - 1} \left(\operatorname{Tr}_{12x} [\operatorname{Tr}_{3y}[A] \operatorname{Tr}_{3y}[A']] - \frac{\operatorname{Tr}_x [\operatorname{Tr}_{123y}[A] \operatorname{Tr}_{123y}[A']]}{d^2} \right)
- \frac{t_4^{(1)} \delta_{pq} \delta_{p'q'}}{d^4 - 1} \left(\operatorname{Tr}_{123x} [\operatorname{Tr}_y[A] \operatorname{Tr}_y[A']] - \frac{\operatorname{Tr}_{12x} [\operatorname{Tr}_{3y}[A] \operatorname{Tr}_{3y}[A']]}{d'} \right)$$
(65)

where $d' = d^2$ if $\mathcal{H}_4 \in \mathcal{H}_k$, and d' = d otherwise. Similarly, $\mathcal{H}_y = \mathcal{H}_4$, $\mathcal{H}_x = \mathcal{H}_0$ if $\mathcal{H}_4 \in \mathcal{H}_j$, and $\mathcal{H}_y = \mathcal{H}_0$, $\mathcal{H}_x = \mathcal{H}_4$ otherwise. In addition, we have

$$t_{1}^{(1)} = \begin{cases} d & \text{if } \mathcal{H}_{2} \in \mathcal{H}_{j} \\ 0 & \text{if } \mathcal{H}_{k} = \mathcal{H}_{2} \\ d^{2} & \text{otherwise} \end{cases}, \quad t_{2}^{(1)} = \begin{cases} d^{2} & \text{if } \mathcal{H}_{2} \in \mathcal{H}_{j} \\ 0 & \text{if } \mathcal{H}_{k} = \mathcal{H}_{2} \\ d & \text{otherwise} \end{cases}, \quad t_{4}^{(1)} = \begin{cases} 1 & \text{if } \mathcal{H}_{2} \in \mathcal{H}_{j}, \text{ and } \mathcal{H}_{3} \in \mathcal{H}_{k} \\ 0 & \text{if } \mathcal{H}_{k} = \mathcal{H}_{1} \\ \frac{1}{d} & \text{otherwise} \end{cases}$$
(66)

$$t_{3}^{(1)} = \begin{cases} d & \text{if } \mathcal{H}_{k} = \mathcal{H}_{3}, \text{ and } \mathcal{H}_{2} \in \mathcal{H}_{l} \\ 1 - d^{2} & \text{if } \mathcal{H}_{k} = \mathcal{H}_{2} \\ \frac{1}{d} & \text{if } \mathcal{H}_{k} = \mathcal{H}_{2} \otimes \mathcal{H}_{3}, \text{ or if } \mathcal{H}_{k} = \mathcal{H}_{3} \otimes \mathcal{H}_{4}, \text{ and } \mathcal{H}_{j} = \mathcal{H}_{2} \end{cases}$$

$$(67)$$

$$t_{3}^{(1)} = \begin{cases} d & \text{if } \mathcal{H}_{k} = \mathcal{H}_{3}, \text{ and } \mathcal{H}_{2} \in \mathcal{H}_{1} \\ d & \text{otherwise} \end{cases}$$

where we can verify that for all 12 possible cases $\sum_{k=1}^{4} \left| \frac{t_k^{(1)}}{(d^4-1)} \right| \leq 1$. Second, let us consider the quantity

$$\Delta\Omega_{jkl}^{(2)} = \operatorname{Tr}_{kl} \left[\operatorname{Tr}_{1j}[\Omega_2] \operatorname{Tr}_{1j}[\Omega'_2] \right] - \frac{\operatorname{Tr}_l \left[\operatorname{Tr}_{12j}[\Omega_2]_{1jk} \operatorname{Tr}[\Omega'_2] \right]}{d_k} \,. \tag{68}$$

Then, for $\mathcal{H}_k \in \{\mathcal{H}_2, \mathcal{H}_3, \mathcal{H}_2 \otimes \mathcal{H}_3, \mathcal{H}_3 \otimes \mathcal{H}_4\}$, the following equality always holds

$$\int d\mu(W) \Delta\Omega_{jkl}^{(2)} = \frac{t_1^{(2)}}{d^2 + 1} \left(\operatorname{Tr}_{123x}[\operatorname{Tr}_y[A]\operatorname{Tr}_y[A']] - \frac{\operatorname{Tr}_{3x}[\operatorname{Tr}_{12y}[A]\operatorname{Tr}_{12y}[A']]}{d^2} \right)
+ \frac{t_2^{(2)}}{d^2 + 1} \left(\operatorname{Tr}_{3x}[\operatorname{Tr}_{12y}[A]\operatorname{Tr}_{12y}[A']] - \frac{\operatorname{Tr}_x[\operatorname{Tr}_{123y}[A]\operatorname{Tr}_{123y}[A']]}{d'} \right)
- \frac{t_3^{(2)}}{d^2 + 1} \left(\operatorname{Tr}_{12x}[\operatorname{Tr}_{3y}[A]\operatorname{Tr}_{3y}[A']] - \frac{\operatorname{Tr}_x[\operatorname{Tr}_{123y}[A]\operatorname{Tr}_{123y}[A']]}{d^2} \right),$$
(69)

where $d' = d^2$ if $\mathcal{H}_4 \in \mathcal{H}_k$, and d' = d otherwise. Similarly, $\mathcal{H}_y = \mathcal{H}_4$, $\mathcal{H}_x = \mathcal{H}_0$ if $\mathcal{H}_4 \in \mathcal{H}_j$, and $\mathcal{H}_y = \mathcal{H}_0$, $\mathcal{H}_x = \mathcal{H}_4$ otherwise. In addition, we now have

$$t_{1}^{(2)} = \begin{cases} 0 & \text{if } \mathcal{H}_{2} \in \mathcal{H}_{j} \\ d & \text{otherwise} \end{cases}, \quad t_{2}^{(2)} = \begin{cases} 0 & \text{if } \mathcal{H}_{2} \in \mathcal{H}_{j}, \text{ or } \mathcal{H}_{k} = \mathcal{H}_{2} \\ \frac{d^{2}+1}{d} & \text{otherwise} \end{cases}, \quad t_{3}^{(2)} = \begin{cases} 1 & \text{if } \mathcal{H}_{2} \in \mathcal{H}_{l}, \text{ and } \mathcal{H}_{k} = \mathcal{H}_{3} \\ \frac{1}{d} & \text{if } \mathcal{H}_{l} = \mathcal{H}_{2}, \text{ and } \mathcal{H}_{k} = \mathcal{H}_{3} \otimes \mathcal{H}_{4} \end{cases}, \quad (70)$$

where we can verify that for all 9 nontrivial cases $\sum_{k=1}^{3} \left| \frac{t_k^{(2)}}{d^2+1} \right| \leq 1$.

Proof. The proof of Eqs. (65), and (69) can be obtain by explicitly integrating each term via (51). In particular, among all possible choices for i, and j, we can find from (65)

$$\int d\mu(W) \left(\text{Tr}_{34} \left[\text{Tr}_{12}[\Omega_{1}] \text{Tr}_{12}[\Omega'_{1}] \right] - \frac{\text{Tr}[\Omega_{1}] \text{Tr}[\Omega'_{1}]}{d^{2}} \right) = \frac{d^{2} \delta_{p_{2} q'_{2}} \delta_{p'_{2} q_{2}}}{d^{4} - 1} \left(\text{Tr}_{234} [\text{Tr}_{1}[\Omega_{2}] \text{Tr}_{1}[\Omega'_{2}]] - \frac{\text{Tr}_{4} [\text{Tr}_{123}[\Omega_{2}] \text{Tr}_{123}[\Omega'_{2}]]}{d^{2}} \right) \\
+ \frac{d \delta_{p_{2} q_{2}} \delta_{p'_{2} q'_{2}}}{d^{4} - 1} \left(\text{Tr}_{4} [\text{Tr}_{123}[\Omega_{2}] \text{Tr}_{123}[\Omega'_{2}]] - \frac{\text{Tr}[\Omega_{2}] \text{Tr}[\Omega'_{2}]}{d} \right) \\
- \frac{\delta_{p_{2} q'_{2}} \delta_{p'_{2} q_{2}}}{d(d^{4} - 1)} \left(\text{Tr}_{23} [\text{Tr}_{14}[\Omega_{2}] \text{Tr}_{14}[\Omega'_{2}]] - \frac{\text{Tr}[\Omega_{2}] \text{Tr}_{14}[\Omega'_{2}]}{d^{2}} \right) \\
- \frac{\delta_{p_{2} q_{2}} \delta_{p'_{2} q'_{2}}}{d(d^{4} - 1)} \left(\text{Tr}_{234} [\text{Tr}_{1}[\Omega_{2}] \text{Tr}_{1}[\Omega'_{2}]] - \frac{\text{Tr}_{23} [\text{Tr}_{14}[\Omega_{2}] \text{Tr}_{14}[\Omega'_{2}]]}{d} \right).$$
(71)

Lemma 7. Let $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \mathcal{H}_3$ be a tripartite Hilbert space of dimension $d = d_1 d_2 d_3$, and let $O_1 = O_A \otimes \mathbb{1}_2 \otimes \mathbb{1}_3$, and $O_1 = \mathbb{1}_1 \otimes O_B \otimes \mathbb{1}_3$ be linear operators on S. Here $\mathbb{1}_i$ indicates the identity over subsystem S_i , so that O_1 and O_2 have no overlapping support. Then for any linear operators $O_A : S_1 \to S_1$, and $O_B : S_2 \to S_2$ we have

$$\operatorname{Tr}_{jk} \left[\operatorname{Tr}_i \left[O_1 \right] \operatorname{Tr}_i \left[O_2 \right] \right] - \frac{\operatorname{Tr}_k \left[\operatorname{Tr}_{ij} \left[O_1 \right] \operatorname{Tr}_{ij} \left[O_2 \right] \right]}{d_j} = 0,$$
 (72)

where Tr_i indicates the partial trace over \mathcal{H}_i , $\operatorname{Tr}_{ij} := \operatorname{Tr}_i \operatorname{Tr}_j$, and where we defined $\mathcal{H}_i \otimes \mathcal{H}_j \otimes \mathcal{H}_k = \mathcal{H}$ such that $\mathcal{H}_j = \mathcal{H}_1, \mathcal{H}_2$ or \mathcal{H}_3 . Moreover, one can always choose $\mathcal{H}_i = \mathcal{H}_0 := \{\mathbf{0}\}$ (or $\mathcal{H}_k = \mathcal{H}_0$), in which case we define the partial trace over \mathcal{H}_0 as $\operatorname{Tr}_0[O] := O$, and $\operatorname{Tr}_{j0}[O] := \operatorname{Tr}_k[O]$.

Proof. Let us show how this equality holds for the specific case when $\mathcal{H}_i = \{0\}$, $\mathcal{H}_j = \mathcal{H}_2$, and $\mathcal{H}_k = \mathcal{H}_1 \otimes \mathcal{H}_3$, and let us remark that all remaining cases follow similarly We have

$$\operatorname{Tr}_{0}[O_{1}]\operatorname{Tr}_{0}[O_{2}] = O_{A} \otimes O_{B} \otimes \mathbb{1}_{3}, \quad \operatorname{Tr}_{2}[O_{1}] = d_{2}O_{A} \otimes \mathbb{1}_{3}, \quad \operatorname{Tr}_{2}[O_{2}] = \operatorname{Tr}_{2}[O_{B}]\mathbb{1}_{1} \otimes \mathbb{1}_{3}, \tag{73}$$

and Eq. (72) becomes

$$\operatorname{Tr}_{123}\left[O_{1}O_{2}\right] - \frac{\operatorname{Tr}_{13}\left[\operatorname{Tr}_{2}\left[O_{1}\right]\operatorname{Tr}_{2}\left[O_{2}\right]\right]}{d_{2}} = \operatorname{Tr}_{123}\left[O_{A} \otimes O_{B} \otimes \mathbb{1}_{3}\right] - \frac{d_{2}\operatorname{Tr}_{2}\left[O_{B}\right]\operatorname{Tr}_{13}\left[O_{A} \otimes \mathbb{1}_{3}\right]}{d_{2}}$$
(74)

$$= d_3 \operatorname{Tr}_1[O_A] \operatorname{Tr}_2[O_B] - \frac{d_2 d_3 \operatorname{Tr}_1[O_A] \operatorname{Tr}_2[O_B]}{d_2}$$
 (75)

$$=0. (76)$$

Supplementary Note 2: Proof of Proposition 1

Here we provide a proof for Proposition 1, which we recall for convenience:

Proposition 1. If θ^j is uniformly distributed on $[-\pi, \pi] \ \forall j$, then for any $\delta \in (0, 1)$, and in the limit that n is large, the probability that $C_G \leq \delta$ is upper bounded by

$$\Pr\left\{C_G \leqslant \delta \mid \forall \delta \in (0,1)\right\} \leqslant \frac{\left(2\pi e\left(1 - \left(1 - \delta\right)^{\frac{1}{n}}\right)\right)^{\frac{n}{2}}}{\sqrt{\pi n}}.\tag{77}$$

For $\delta \in (1/2, 1]$, the probability that $C_L \leqslant \delta$ is lower bounded by

$$\Pr\left\{C_L \leqslant \delta \mid \forall \delta \in (1/2, 1]\right\} \geqslant \frac{(2\delta - 1)^2}{(2\delta - 1)^2 + \frac{1}{2n}} \xrightarrow{n \to \infty} 1. \tag{78}$$

Proposition 1 formalizes the narrow gorge phenomenon shown in Fig. 2 of the main text for the warm-up example. Specifically, it bounds the volume of parameter space that is trainable in the sense that the cost deviates from its maximum value of one. In the following proof, it is helpful to define the trainable region for the global and local cost as $A_{\delta}^G := \{: C_G(\theta) \leq \delta\}$ and $A_{\delta}^L := \{\theta : C_L(\theta) \leq \delta\}$.

Proof. Let us first consider the global cost function

$$C_G = \text{Tr}[O_G V(\boldsymbol{\theta}) | \mathbf{0} \rangle \langle \mathbf{0} | V(\boldsymbol{\theta})^{\dagger}], \tag{79}$$

with $O_G = \mathbb{1} - |\mathbf{0}\rangle\langle\mathbf{0}|$, and with $V(\boldsymbol{\theta}) = \bigotimes_{j=1}^n e^{-i\theta^j \sigma_x^{(j)}/2}$. The probability that C_G is in the trainable region is

$$\Pr(A_{\delta}^{G}) = \frac{1}{(2\pi)^{n}} \int_{\prod_{j=1}^{n} \cos^{2}(\theta^{j}/2) \geqslant 1-\delta} d\theta \leqslant \frac{1}{\pi^{n}} \int_{\|u\|^{2} \leqslant n(1-(1-\delta)^{\frac{1}{n}})} du \prod_{j=1}^{n} \frac{1}{\sqrt{1-u_{j}^{2}}},$$
(80)

where the inequality of arithmetic and geometric means (AM-GM inequality) has been used and $u_j = \sin(\theta^j/2) \in [-1,1]$. As $n \to \infty$, the radius of the integration ball vanishes and the integrand can be replaced by 1. Since the AM-GM inequality is tight for vanishing arguments, we obtain the fact that $\lim_{n\to\infty} \pi^n \Pr(A_\delta^G)/V_n(R_n) = 1$, where $V_n(R)$ is the volume of the n-ball of radius R and $R_n := \sqrt{n(1-(1-\delta)^{\frac{1}{n}})}$. Application of Stirling's approximation yields, $\pi^{-n}V_n(R_n) \leqslant \frac{1}{\sqrt{\pi n}} \left(2\pi e(1-(1-\delta)^{1/n})\right)^{n/2}$ for any $\delta \in (0,1)$, which exhibits an exponential decay with n. Now consider the local cost function C_L given by

$$C_L = \operatorname{Tr}\left[O_L V(\boldsymbol{\theta})|\mathbf{0}\rangle\langle\mathbf{0}|V(\boldsymbol{\theta})^{\dagger}\right], \quad \text{with} \quad O_L = \mathbb{1} - \frac{1}{n} \sum_{j=1}^n |0\rangle\langle 0|_j \otimes \mathbb{1}_{\overline{j}},$$
(81)

and where $\mathbb{1}_{\bar{j}}$ is the identity on all qubits except qubit j. To show the dependence of the result on the range of local cost function values, we write a parametrized local cost function $C_L(\theta;\lambda) := 1 - \frac{1}{\lambda n} \sum_{j=1}^n \cos^2 \frac{\theta_j}{2}$ and define $A_{\delta}^L := \{\theta : C_L(\theta;\lambda) \leq \delta\}$. C_L in the main text is obtained for $\lambda = 1$. The parameter λ is introduced to show that the range of validity of the inequality is dependent on the cost function. For δ in the interval $\delta \in (1 - (2\lambda)^{-1}, 1]$,

$$\Pr\left(A_{\delta}^{L}\right) = \Pr\left(\left\{\theta : \frac{1}{\lambda n} \sum_{j=1}^{n} \cos^{2} \frac{\theta^{j}}{2} \ge 1 - \delta\right\}\right) \geqslant \frac{(1 - 2\lambda(1 - \delta))^{2}}{\frac{1}{2n} + (1 - 2\lambda(1 - \delta))^{2}}$$
(82)

which tends to 1 as $n \to \infty$. The inequality follows from the Paley-Zygmund inequality [43] in the form

$$P(X \ge rE(X)) \ge \frac{(1-r)^2 E(X)^2}{\text{Var}X + (1-r)^2 E(X)^2}$$
(83)

which holds for random variables $X \geq 0$ and scalar r with $0 \leqslant r \leqslant 1$. In particular, (82) follows by taking $X = \frac{1}{n\lambda} \sum_{j=1}^{n} \cos^2 \frac{\theta j}{2}$ and $r = 2\lambda(1-\delta)$, so that r varies from 1 to 0 as δ varies from $1-(2\lambda)^{-1}$ to 1.

Supplementary Note 3: Proof of Proposition 2

Let us first recall that in the main text we analyze cost functions C which can be expressed as the expectation value of a given observable O as

$$C = \text{Tr} \left[OV(\boldsymbol{\theta}) \rho V^{\dagger}(\boldsymbol{\theta}) \right] , \tag{84}$$

where $V(\theta)$ is a parametrized quantum gate sequence and ρ is a general input mixed quantum state on n qubits. Here we provide a proof for Proposition 2, which we recall for convenience:

Proposition 2. The average of the partial derivative of any cost function of the form (84) with respect to a parameter θ^{ν} in a block W of the ansatz $V(\theta)$ is

$$\langle \partial_{\nu} C \rangle_{V} = 0, \tag{85}$$

provided that either W_A or W_B form a 1-design.

As discussed in the main text, we employ an Alternating Layered Ansatz, where each layer is composed of m-qubits gates or "blocks". In particular, each block $W_{kl}(\boldsymbol{\theta}_{kl})$ in $V(\boldsymbol{\theta})$ can be written as a product of ζ_{kl} independent gates from a gate alphabet $\mathcal{A} = \{G_{\mu}(\boldsymbol{\theta})\}$ as

$$W_{kl}(\boldsymbol{\theta}_{kl}) = G_{\zeta_{kl}}(\theta_{kl}^{\zeta_{kl}}) \dots G_{\nu}(\theta_{kl}^{\nu}) \dots G_{1}(\theta_{kl}^{1}), \qquad (86)$$

where θ_{kl}^{ν} are continuous parameter, and where $G_{\nu}(\theta_{kl}^{\nu}) = R_{\nu}(\theta_{kl}^{\nu})Q_{\nu}$ with Q_{ν} an unparameterized gate, and $R_{\nu}(\theta_{kl}^{\nu}) = e^{-i\theta_{kl}^{\nu}\sigma_{\nu}/2}$ such that σ_{ν} is a Pauli operator.

Consider now a block $W_{kl}(\boldsymbol{\theta}_{kl})$ in the l-th layer of the ansatz. For the rest of this Supplementary Information we simply use the notation W when referring to this particular block. First, let S_w denote the m-qubit subsystem that contains the qubits W acts on, and let $S_{\overline{w}}$ be the (n-m) subsystem on which W acts trivially, with \mathcal{H}_w , and $\mathcal{H}_{\overline{w}}$ their respective associated Hilbert spaces. Then, consider a given trainable parameter θ^{ν} in W, such that we can express $W = W_B W_A$, with

$$W_B = \prod_{\mu=1}^{\nu-1} G_{\mu}(\theta^{\mu}), \text{ and } W_A = \prod_{\mu=\nu}^{\zeta} G_{\mu}(\theta^{\mu}).$$
 (87)

Then, we recall that we have defined the forward light-cone \mathcal{L} of W as all gates with at least one input qubit causally connected to the output qubits of W. We can then define $S_{\mathcal{L}}$ as the subsystem of all qubits in \mathcal{L} , and $\mathcal{H}_{\mathcal{L}}$ as its associated Hilbert space. Without loss of generality, the trainable gate sequence can be expressed as

$$V(\boldsymbol{\theta}) = V_L(\mathbb{1}_{\overline{w}} \otimes W)V_R, \qquad (88)$$

where $\mathbb{1}_{\overline{w}}$ indicates the identity in $\mathcal{H}_{\overline{w}}$, and where we assume without loss of generality that V_R contains the gates in \mathcal{L} and all the blocks W_{kL} in the last layer of $V(\boldsymbol{\theta})$.

Proof. The partial derivative of W with respect to the angle θ_{ν} is given by

$$\partial_{\nu}W = W_A \left(-\frac{i}{2}\sigma_{\nu} \right) W_B \,, \tag{89}$$

where here σ_{ν} is an operator $\sigma_{\nu}: \mathcal{H}_w \to \mathcal{H}_w$, which acts non-trivially on a qubit given qubit j in \mathcal{H}_w , i.e., $\sigma_{\nu}:=(\sigma_{\nu})_j\otimes \mathbb{1}_{\overline{j}}$. Hence, by means of Eqs. (89) and (88) we have

$$\begin{split} \partial_{\nu} C = & \text{Tr} \left[O \left(\partial_{\nu} V (\boldsymbol{\theta}) \right) \rho V^{\dagger} (\boldsymbol{\theta}) + V (\boldsymbol{\theta}) \rho \left(\partial_{\nu} V^{\dagger} (\boldsymbol{\theta}) \right) \right] \\ = & \text{Tr} \left[O V_{R} \left(\mathbb{1}_{\overline{w}} \otimes W_{A} \right) \left(\mathbb{1}_{\overline{w}} \otimes \left(-\frac{i}{2} \sigma_{\nu} \right) \right) \left(\mathbb{1}_{\overline{w}} \otimes W_{B} \right) V_{L} \rho V_{L}^{\dagger} \left(\mathbb{1}_{\overline{w}} \otimes W_{B}^{\dagger} W_{A}^{\dagger} \right) V_{R}^{\dagger} \right] \\ + & \text{Tr} \left[O V_{R} \left(\mathbb{1}_{\overline{w}} \otimes W_{A} W_{B} \right) V_{L} \rho V_{L}^{\dagger} \left(\mathbb{1}_{\overline{w}} \otimes W_{B}^{\dagger} \right) \left(\mathbb{1}_{\overline{w}} \otimes \left(+\frac{i}{2} \sigma_{\nu} \right) \right) \left(\mathbb{1}_{\overline{w}} \otimes W_{A}^{\dagger} \right) V_{R}^{\dagger} \right] . \end{split}$$

Which can me simplified as

$$\partial_{\nu}C = \frac{i}{2} \operatorname{Tr} \left[(\mathbb{1}_{\overline{w}} \otimes W_B) V_L \rho V_L^{\dagger} \left(\mathbb{1}_{\overline{w}} \otimes W_B^{\dagger} \right) \left[\mathbb{1}_{\overline{w}} \otimes \sigma_{\nu}, \left(\mathbb{1}_{\overline{w}} \otimes W_A^{\dagger} \right) V_R^{\dagger} O V_R \left(\mathbb{1}_{\overline{w}} \otimes W_A \right) \right] \right], \tag{90}$$

or equivalently, as

$$\partial_{\nu}C = -\frac{i}{2} \operatorname{Tr} \left[\left(\mathbb{1}_{\overline{w}} \otimes W_{A}^{\dagger} \right) V_{R}^{\dagger} O V_{R} \left(\mathbb{1}_{\overline{w}} \otimes W_{A} \right) \left[\mathbb{1}_{\overline{w}} \otimes \sigma_{\nu}, \left(\mathbb{1}_{\overline{w}} \otimes W_{B} \right) V_{L} \rho V_{L}^{\dagger} \left(\mathbb{1}_{\overline{w}} \otimes W_{B}^{\dagger} \right) \right] \right]. \tag{91}$$

In order to compute the expectation value $\langle \partial_{\nu} C \rangle_{V}$ we need to consider three different scenarios: (1) when only W_{A} is a 1-design; (2) when only W_{B} is a 1-design; and (3) when both W_{A} and W_{B} form 1-designs. We first consider the case when W_{A} is a 1-design. Since W_{A} , W_{B} , V_{R} and V_{L} are independent, we can compute the expectation value over the ansatz as $\langle \partial_{\nu} C \rangle_{V} = \langle \langle \partial_{\nu} C \rangle_{W_{A}} \rangle_{V_{L},W_{B},V_{R}}$. From (90) and the definition of a 1-design in (49), we can compute

$$\langle \partial_{\nu} C \rangle_{W_{A}} = -\frac{i}{2} \operatorname{Tr} \left[(\mathbb{1}_{\overline{w}} \otimes W_{B}) V_{L} \rho V_{L}^{\dagger} \left(\mathbb{1}_{\overline{w}} \otimes W_{B}^{\dagger} \right) \left[\mathbb{1}_{\overline{w}} \otimes \sigma_{\nu}, \int d\mu(W_{A}) \left(\mathbb{1}_{\overline{w}} \otimes W_{A} \right) V_{R}^{\dagger} O V_{R} \left(\mathbb{1}_{\overline{w}} \otimes W_{A}^{\dagger} \right) \right] \right]$$

$$= -\frac{i}{2} \operatorname{Tr} \left[\left(\mathbb{1}_{\overline{w}} \otimes W_{B} \right) V_{L} \rho V_{L}^{\dagger} \left(\mathbb{1}_{\overline{w}} \otimes W_{B}^{\dagger} \right) \left[\mathbb{1}_{\overline{w}} \otimes \sigma_{\nu}, \frac{1}{2^{m}} \operatorname{Tr}_{w} [V_{R}^{\dagger} O V_{R}] \otimes \mathbb{1}_{w} \right] \right]$$

$$= 0, \tag{92}$$

where in the second equality we used Lemma 4.

On the other hand, if W_B is a 1-design, we can now employ (91) to get

$$\langle \partial_{\nu} C \rangle_{W_{B}} = -\frac{i}{2} \operatorname{Tr} \left[\left(\mathbb{1}_{\overline{w}} \otimes W_{A}^{\dagger} \right) V_{R}^{\dagger} O V_{R} \left(\mathbb{1}_{\overline{w}} \otimes W_{A} \right) \left[\mathbb{1}_{\overline{w}} \otimes \sigma_{\nu}, \int d\mu(W_{B}) \left(\mathbb{1}_{\overline{w}} \otimes W_{B} \right) V_{L} \rho V_{L}^{\dagger} \left(\mathbb{1}_{\overline{w}} \otimes W_{B}^{\dagger} \right) \right] \right]$$

$$= -\frac{i}{2} \operatorname{Tr} \left[\left(\mathbb{1}_{\overline{w}} \otimes W_{A}^{\dagger} \right) V_{R}^{\dagger} O V_{R} \left(\mathbb{1}_{\overline{w}} \otimes W_{A} \right) \left[\mathbb{1}_{\overline{w}} \otimes \sigma_{\nu}, \frac{1}{2^{m}} \operatorname{Tr}_{w} \left[V_{L} \rho V_{L}^{\dagger} \right] \otimes \mathbb{1}_{w} \right] \right]$$

$$= 0,$$

$$(93)$$

which follows from the same argument used to derive (92). Finally, from Eqs. (92) and (93), we have $\langle \partial_{\nu} C \rangle_{V} = 0$ ($\forall V_{L}, V_{R}$) if W_{A} and W_{B} are both 1-designs.

Supplementary Note 4: Variance of the cost function partial derivative

In this section, we derive the formula for the variance of the cost function gradient. Namely,

$$\langle (\partial_{\nu}C)^{2} \rangle_{V} = \frac{2^{m-1} \text{Tr}[\sigma_{\nu}^{2}]}{(2^{2m}-1)^{2}} \sum_{\substack{pq \ p'q'}} \left\langle \Delta \Omega_{pq}^{p'q'} \right\rangle_{V_{R}} \left\langle \Delta \Psi_{pq}^{p'q'} \right\rangle_{V_{L}}, \tag{94}$$

with

$$\Delta\Omega_{pq}^{p'q'} = \text{Tr}[\Omega_{qp}\Omega_{q'p'}] - \frac{\text{Tr}[\Omega_{qp}]\text{Tr}[\Omega_{q'p'}]}{2^m}, \qquad (95)$$

$$\Delta \Psi_{\boldsymbol{p}\boldsymbol{q}}^{\boldsymbol{p}'\boldsymbol{q}'} = \text{Tr}[\Psi_{\boldsymbol{p}\boldsymbol{q}}\Psi_{\boldsymbol{p}'\boldsymbol{q}'}] - \frac{\text{Tr}[\Psi_{\boldsymbol{p}\boldsymbol{q}}]\text{Tr}[\Psi_{\boldsymbol{p}'\boldsymbol{q}'}]}{2^m}, \qquad (96)$$

and where

$$\Omega_{qp} = \text{Tr}_{\overline{w}} \left[(|p\rangle \langle q| \otimes \mathbb{1}_w) V_R^{\dagger} O V_R \right] , \qquad (97)$$

$$\Psi_{pq} = \text{Tr}_{\overline{w}} \left[(|q\rangle \langle p| \otimes \mathbb{1}_w) V_L^{\dagger} \rho V_L \right]. \tag{98}$$

Proof. As shown in the previous section, $\langle \partial_{\nu} C \rangle_{V} = 0$ when either W_{B} or W_{A} of (87) are 1-designs. Hence, we can compute the variance of $\partial_{\nu} C$ as $\text{Var}[\partial_{\nu} C] = \langle (\partial_{\nu} C)^{2} \rangle_{V} - \langle \partial_{\nu} C \rangle_{V}^{2} = \langle (\partial_{\nu} C)^{2} \rangle_{V}$. From (91) and Lemma 5 we have

$$(\partial_{\nu}C)^{2} = -\frac{1}{4} \sum_{\substack{\boldsymbol{p},\boldsymbol{q} \\ \boldsymbol{p}',\boldsymbol{q}'}} \operatorname{Tr} \left[W_{A} \Omega_{\boldsymbol{q}\boldsymbol{p}} W_{A}^{\dagger} \Gamma_{\boldsymbol{p}\boldsymbol{q}} \right] \operatorname{Tr} \left[W_{A} \Omega_{\boldsymbol{q}'\boldsymbol{p}'} W_{A}^{\dagger} \Gamma_{\boldsymbol{p}'\boldsymbol{q}'} \right], \tag{99}$$

with

$$\Gamma_{\boldsymbol{p}\boldsymbol{q}} = \operatorname{Tr}_{\overline{w}} \left[(|\boldsymbol{q}\rangle\langle\boldsymbol{p}| \otimes \mathbb{1}_{w}) \left[\mathbb{1}_{\overline{w}} \otimes \sigma_{\nu}, (\mathbb{1}_{\overline{w}} \otimes W_{B}) V_{L} \rho V_{L}^{\dagger} (\mathbb{1}_{\overline{w}} \otimes W_{B}^{\dagger}) \right] \right]
= \operatorname{Tr}_{\overline{w}} \left[[\mathbb{1}_{\overline{w}} \otimes \sigma_{\nu}, (\mathbb{1}_{\overline{w}} \otimes W_{B}) (|\boldsymbol{q}\rangle\langle\boldsymbol{p}| \otimes \mathbb{1}_{w}) V_{L} \rho V_{L}^{\dagger} (\mathbb{1}_{\overline{w}} \otimes W_{B}^{\dagger}) \right] \right]
= \left[\sigma_{\nu}, W_{B} \operatorname{Tr}_{\overline{w}} [(|\boldsymbol{q}\rangle\langle\boldsymbol{p}| \otimes \mathbb{1}_{w}) V_{L} \rho V_{L}^{\dagger}] W_{B}^{\dagger} \right]
= \left[\sigma_{\nu}, W_{B} \Psi_{\boldsymbol{p}\boldsymbol{q}} W_{B}^{\dagger} \right] .$$
(100)

As previously mentioned, if W_A , W_B , V_R and V_L are independent, the expectation value of (99) can be computed as $\langle (\partial_{\nu}C)^2 \rangle_V = \langle (\partial_{\nu}C)^2 \rangle_{V_L,W_B,W_A,V_R}$. In addition, if W_A is a 2-design, we get from Lemma 3

$$\langle (\partial_{\nu}C)^{2} \rangle_{W_{A}} = -\frac{1}{4} \sum_{\substack{\boldsymbol{p},\boldsymbol{q} \\ \boldsymbol{p}',\boldsymbol{q}'}} \int d\mu(W_{A}) \operatorname{Tr} \left[W_{A} \Omega_{\boldsymbol{q}\boldsymbol{p}} W_{A}^{\dagger} \Gamma_{\boldsymbol{p}\boldsymbol{q}} \right] \operatorname{Tr} \left[W_{A} \Omega_{\boldsymbol{q}'\boldsymbol{p}'} W_{A}^{\dagger} \Gamma_{\boldsymbol{p}'\boldsymbol{q}'} \right]$$

$$= -\frac{1}{4} \sum_{\substack{\boldsymbol{p},\boldsymbol{q} \\ \boldsymbol{p}',\boldsymbol{q}'}} \left(\frac{1}{2^{2m}-1} \left(\operatorname{Tr} [\Omega_{\boldsymbol{q}\boldsymbol{p}}] \operatorname{Tr} [\Gamma_{\boldsymbol{p}\boldsymbol{q}}] \operatorname{Tr} [\Gamma_{\boldsymbol{p}'\boldsymbol{p}'}] \operatorname{Tr} [\Gamma_{\boldsymbol{p}'\boldsymbol{q}'}] + \operatorname{Tr} [\Omega_{\boldsymbol{q}\boldsymbol{p}} \Omega_{\boldsymbol{q}'\boldsymbol{p}'}] \operatorname{Tr} [\Gamma_{\boldsymbol{p}\boldsymbol{q}} \Gamma_{\boldsymbol{p}'\boldsymbol{q}'}] \right)$$

$$- \frac{1}{2^{m}(2^{2m}-1)} \left(\operatorname{Tr} [\Omega_{\boldsymbol{q}\boldsymbol{p}} \Omega_{\boldsymbol{q}'\boldsymbol{p}'}] \operatorname{Tr} [\Gamma_{\boldsymbol{p}\boldsymbol{q}}] \operatorname{Tr} [\Gamma_{\boldsymbol{p}'\boldsymbol{q}'}] + \operatorname{Tr} [\Omega_{\boldsymbol{q}\boldsymbol{p}}] \operatorname{Tr} [\Omega_{\boldsymbol{q}'\boldsymbol{p}'}] \operatorname{Tr} [\Gamma_{\boldsymbol{p}\boldsymbol{q}} \Gamma_{\boldsymbol{p}'\boldsymbol{q}'}] \right)$$

$$= -\frac{1}{4(2^{2m}-1)} \sum_{\substack{\boldsymbol{p},\boldsymbol{q} \\ \boldsymbol{p}',\boldsymbol{q}'}} \left(\operatorname{Tr} [\Omega_{\boldsymbol{q}\boldsymbol{p}} \Omega_{\boldsymbol{q}'\boldsymbol{p}'}] - \frac{1}{2^{m}} \operatorname{Tr} [\Omega_{\boldsymbol{q}\boldsymbol{p}}] \operatorname{Tr} [\Omega_{\boldsymbol{q}'\boldsymbol{p}'}] \right) \operatorname{Tr} [\Gamma_{\boldsymbol{p}\boldsymbol{q}} \Gamma_{\boldsymbol{p}'\boldsymbol{q}'}], \tag{101}$$

where in the third equality we used the fact that the trace of a commutator is zero: $\text{Tr}[\Gamma_{pq}] = 0$. If W_B is also a 2-design, then from (101) we need to compute the following expectation value

$$\langle (\partial_{\nu}C)^{2} \rangle_{W_{B},W_{A}} = -\frac{1}{4(2^{2m}-1)} \sum_{\substack{\boldsymbol{p},\boldsymbol{q} \\ \boldsymbol{p}',\boldsymbol{q}'}} \left(\operatorname{Tr}[\Omega_{\boldsymbol{q}\boldsymbol{p}}\Omega_{\boldsymbol{q}'\boldsymbol{p}'}] - \frac{1}{2^{m}} \operatorname{Tr}[\Omega_{\boldsymbol{q}\boldsymbol{p}}] \operatorname{Tr}[\Omega_{\boldsymbol{q}'\boldsymbol{p}'}] \right) \int d\mu(W_{B}) \operatorname{Tr}[\Gamma_{\boldsymbol{p}\boldsymbol{q}}\Gamma_{\boldsymbol{p}'\boldsymbol{q}'}]. \tag{102}$$

Let us first note that

$$\Gamma_{\boldsymbol{p}\boldsymbol{q}}\Gamma_{\boldsymbol{p}'\boldsymbol{q}'} = \left[\sigma_{\nu}, W_{B}\Psi_{\boldsymbol{p}\boldsymbol{q}}W_{B}^{\dagger}\right] \left[\sigma_{\nu}, W_{B}\Psi_{\boldsymbol{p}'\boldsymbol{q}'}W_{B}^{\dagger}\right]
= 2\left(\sigma_{\nu}W_{B}\Psi_{\boldsymbol{p}\boldsymbol{q}}W_{B}^{\dagger}\sigma_{\nu}W_{B}\Psi_{\boldsymbol{p}'\boldsymbol{q}'}W_{B}^{\dagger}\right) - 2\left(W_{B}\sigma_{\nu}^{2}W_{B}^{\dagger}\Psi_{\boldsymbol{p}\boldsymbol{q}}\Psi_{\boldsymbol{p}'\boldsymbol{q}'}\right). \tag{103}$$

This result can be used along with Lemmas 1 and 2 to compute the integral in (103) as

$$\int d\mu(W_B) \operatorname{Tr}[\Gamma_{\boldsymbol{p}\boldsymbol{q}}\Gamma_{\boldsymbol{p'}\boldsymbol{q'}}] = 2 \int d\mu(W_B) \operatorname{Tr}\left[\sigma_{\nu}W_B\Psi_{\boldsymbol{p}\boldsymbol{q}}W_B^{\dagger}\sigma_{\nu}W_B\Psi_{\boldsymbol{p'}\boldsymbol{q'}}W_B^{\dagger}\right]
- 2 \int d\mu(W_B) \operatorname{Tr}\left[W_B\sigma_{\nu}^2W_B^{\dagger}\Psi_{\boldsymbol{p}\boldsymbol{q}}\Psi_{\boldsymbol{p'}\boldsymbol{q'}}\right]
= -\frac{2^{m+1}}{2^{2m}-1} \operatorname{Tr}[\sigma_{\nu}^2] \left(\operatorname{Tr}[\Psi_{\boldsymbol{p}\boldsymbol{q}}\Psi_{\boldsymbol{p'}\boldsymbol{q'}}] - \frac{1}{2^m} \operatorname{Tr}[\Psi_{\boldsymbol{p}\boldsymbol{q}}] \operatorname{Tr}[\Psi_{\boldsymbol{p'}\boldsymbol{q'}}]\right),$$
(104)

where we used the fact that σ_{ν} is a Pauli operator, and hence its trace is equal to zero.

Then, combining Eqs. (103) and (104), we obtain

$$\langle (\partial_{\nu}C)^{2} \rangle_{V} = \frac{2^{m-1} \text{Tr}[\sigma_{\nu}^{2}]}{(2^{2m}-1)^{2}} \sum_{\substack{pq \ p'q'}} \left\langle \Delta \Omega_{pq}^{p'q'} \right\rangle_{V_{R}} \left\langle \Delta \Psi_{pq}^{p'q'} \right\rangle_{V_{L}}. \tag{105}$$

Supplementary Note 5: Variance of the cost function partial derivative for a single layer of the Alternating Layered Ansatz

In this section we explicitly evaluate Eqs. (94)–(96) for the special case when $V(\theta)$ is composed of a single layer of the Alternating Layered Ansatz. This case is a generalization of the warm-up example of the main text, and constitutes the first step towards our main theorems. In particular, we remark that the tools employed here are the same as the ones used to derive our main result.

A. Variance of global cost function partial derivative

Let us first recall that the global cost function is $C_G = 1 - \text{Tr}\left[OV\rho V^{\dagger}\right]$, where $O = \bigotimes_{k=1}^{\xi} \widehat{O}_k$, and where $V(\theta)$ is given by a single layer of the Alternating Layered Ansatz, i.e., $V(\theta) = \bigotimes_{k=1}^{\xi} W_{k1}\left(\theta_k\right)$. Moreover, we recall that we assume without loss of generality that V_R contains the gates in \mathcal{L} and all the blocks W_{k1} in the last (and in this case only) layer of $V(\theta)$. The latter means that here $V_L = \mathbb{1}$, and $V_R = \mathbb{1}_h \otimes \left(\bigotimes_{k \neq h} W_{k1}\left(\theta_k\right)\right)$. In addition, for simplicity, we have defined $W_{k1} := W_k$. Here, ξ is the total number of blocks so that $n = \xi m$, and we assume that the angle θ_{ν} we want to train is in the h-th block W_h . First, let us compute Ω_{qp} . From (97), we obtain

$$\Omega_{qp} = \widehat{O}_h \prod_{k \neq h}^{\xi} \text{Tr} \left[W_k^{\dagger} \widehat{O}_k W_k | \boldsymbol{p}_k \rangle \langle \boldsymbol{q}_k | \right].$$
 (106)

Replacing this result in Eq. (95) and employing Lemma 3 ($\xi - 1$)-times results in

$$\begin{split} \left\langle \Delta \Omega_{\boldsymbol{p}\boldsymbol{q}}^{\boldsymbol{p}'\boldsymbol{q}'} \right\rangle_{V_R} = & \frac{1}{(2^{2m}-1)^{\xi-1}} \left(\mathrm{Tr} \left[\widehat{O}_h^2 \right] - \frac{1}{2^m} \mathrm{Tr} \left[\widehat{O}_h \right]^2 \right) \\ & \times \prod_{k \neq h}^{\xi} \left(\delta_{(\boldsymbol{p},\boldsymbol{q})_{S_k}} \delta_{(\boldsymbol{p}',\boldsymbol{q}')_{S_k}} \left(\mathrm{Tr} \left[\widehat{O}_k \right]^2 - \frac{1}{2^m} \mathrm{Tr} \left[\widehat{O}_k^2 \right] \right) + \delta_{(\boldsymbol{p}',\boldsymbol{q})_{S_k}} \delta_{(\boldsymbol{p},\boldsymbol{q}')_{S_k}} \left(\mathrm{Tr} \left[\widehat{O}_k^2 \right] - \frac{1}{2^m} \mathrm{Tr} \left[\widehat{O}_k \right]^2 \right) \right) \,. \end{split}$$

Now, let us consider \widehat{O}_k $(k = 1, 2, \dots, \xi)$ to be rank-1 projector, i.e. $\operatorname{Tr}\left[\widehat{O}_k\right] = \operatorname{Tr}\left[\widehat{O}_k^2\right] = \operatorname{rank}\left[\widehat{O}_k\right] = 1$. Therefore, we can obtain

$$\left\langle \Delta \Omega_{\boldsymbol{p}\boldsymbol{q}}^{\boldsymbol{p}'\boldsymbol{q}'} \right\rangle_{V_R} = \frac{1}{(2^{2m} - 1)^{\xi - 1}} \left(1 - \frac{1}{2^m} \right)^{\xi} \prod_{k \neq h}^{\xi} \left(\delta_{(\boldsymbol{p}, \boldsymbol{q})_{S_k}} \delta_{(\boldsymbol{p}', \boldsymbol{q}')_{S_k}} + \delta_{(\boldsymbol{p}', \boldsymbol{q})_{S_k}} \delta_{(\boldsymbol{p}, \boldsymbol{q}')_{S_k}} \right). \tag{107}$$

Next, let us consider Ψ_{pq} in (98). Here, we can set $V_L = 1$, which leads to $\Psi_{pq} = \text{Tr}_{\overline{h}}[(|p\rangle\langle q|\otimes 1_h)\rho]$. Note that any quantum state ρ can be always written as

$$\rho = \sum_{\lambda} p_{\lambda} |\psi_{\lambda}\rangle\langle\psi_{\lambda}|, \quad \text{with} \quad |\psi_{\lambda}\rangle = \sum_{\alpha^{\lambda}} c_{\alpha^{\lambda}} |\alpha_{1}^{\lambda}\rangle \otimes \cdots \otimes |\alpha_{h}^{\lambda}\rangle \otimes \cdots \otimes |\alpha_{\xi}^{\lambda}\rangle,$$
(108)

where $\alpha := \alpha_1 \cdots \alpha_{\xi}$, and where α_i are bitstrings of length m. Hence we find

$$\Psi_{pq} = \sum_{\lambda} p_{\lambda} \sum_{\boldsymbol{\alpha}^{\lambda}, \boldsymbol{\alpha}'^{\lambda}} c_{\boldsymbol{\alpha}^{\lambda}} c_{\boldsymbol{\alpha}'^{\lambda}}^{*} \left(\prod_{k \neq h}^{\xi} \delta_{(\boldsymbol{q}, \boldsymbol{\alpha}^{\lambda})_{k}} \delta_{(\boldsymbol{p}, \boldsymbol{\alpha}'^{\lambda})_{S_{k}}} \right) |\boldsymbol{\alpha}_{h}^{\lambda}\rangle \langle \boldsymbol{\alpha'}_{h}^{\lambda}|.$$

$$(109)$$

Then, since $V_L = 1$, we have $\left\langle \Delta \Psi_{pq}^{p'q'} \right\rangle_{V_L} = \Delta \Psi_{pq}^{p'q'}$, and we can use (109) to get

$$\Delta\Psi_{\mathbf{p}q}^{\mathbf{p}'\mathbf{q}'} = \sum_{\lambda,\lambda'} p_{\lambda} p_{\lambda'} \sum_{\substack{\alpha^{\lambda},\alpha'^{\lambda} \\ \beta^{\lambda'},\beta'^{\lambda'}}} c_{\alpha^{\lambda}} c_{\beta^{\lambda'}}^{*} c_{\beta'^{\lambda'}}^{*} \left(\prod_{k\neq h}^{\xi} \delta_{(\mathbf{q},\alpha^{\lambda})_{S_{k}}} \delta_{(\mathbf{p},\alpha'^{\lambda})_{S_{k}}} \delta_{(\mathbf{q}',\beta^{\lambda'})_{S_{k}}} \delta_{(\mathbf{p}',\beta'^{\lambda'})_{S_{k}}} \right) \times \left(\delta_{(\alpha'^{\lambda},\beta^{\lambda'})_{S_{h}}} \delta_{(\alpha^{\lambda},\beta'^{\lambda'})_{S_{h}}} - \frac{1}{2^{m}} \delta_{(\alpha^{\lambda},\alpha'^{\lambda})_{S_{h}}} \delta_{(\beta^{\lambda'},\beta'^{\lambda'})_{S_{h}}} \right). \tag{110}$$

Finally, from (107), (110), and the fact that $\text{Tr}\left[\sigma_{\nu}^{2}\right]=2^{m}$, we obtain

$$\begin{aligned} \operatorname{Var}\left[\partial_{\nu}C_{G}\right] &= \frac{2^{2m-1}}{(2^{2m}-1)^{2}(2^{2m}-1)^{\xi-1}} \left(1-\frac{1}{2^{m}}\right)^{\xi} \sum_{\lambda,\lambda'} p_{\lambda}p_{\lambda'} \sum_{\substack{\alpha^{\lambda},\alpha'^{\lambda} \\ \beta^{\lambda'},\beta'^{\lambda'}}} c_{\alpha^{\lambda}}c_{\alpha'^{\lambda}}^{*}c_{\beta^{\lambda'}}c_{\beta'^{\lambda'}}^{*} \\ &\times \left(\delta_{(\alpha'^{\lambda},\beta^{\lambda'})_{S_{h}}} \delta_{(\alpha^{\lambda},\beta'^{\lambda'})_{S_{h}}} - \frac{1}{2^{m}} \delta_{(\alpha^{\lambda},\alpha'^{\lambda})_{S_{h}}} \delta_{(\beta^{\lambda'},\beta'^{\lambda'})_{S_{h}}}\right) \prod_{k\neq h} \left(\delta_{(\alpha^{\lambda},\alpha'^{\lambda})_{S_{k}}} \delta_{(\beta^{\lambda'},\beta'^{\lambda'})_{S_{k}}} + \delta_{(\alpha^{\lambda},\beta'^{\lambda'})_{S_{k}}} \delta_{(\alpha'^{\lambda},\beta^{\lambda'})_{S_{k}}}\right), \end{aligned}$$

where we used the fact that

$$\sum_{\substack{\mathbf{p}\mathbf{q}\\\mathbf{p}'\mathbf{q}'}} \left(\prod_{k\neq h}^{\xi} \left(\delta_{(\mathbf{p},\mathbf{q})_{S_k}} \delta_{(\mathbf{p}',\mathbf{q}')_{S_k}} + \delta_{(\mathbf{p}',\mathbf{q})_{S_k}} \delta_{(\mathbf{p},\mathbf{q}')_{S_k}} \right) \delta_{(\mathbf{q},\boldsymbol{\alpha}^{\lambda})_{S_k}} \delta_{(\mathbf{p},\boldsymbol{\alpha}'^{\lambda})_{S_k}} \delta_{(\mathbf{q}',\boldsymbol{\beta}^{\lambda'})_{S_k}} \delta_{(\mathbf{p}',\boldsymbol{\beta}'^{\lambda'})_{S_k}} \right) \\
= \prod_{k\neq h} \left(\delta_{(\boldsymbol{\alpha}^{\lambda},\boldsymbol{\alpha}'^{\lambda})_{S_k}} \delta_{(\boldsymbol{\beta}^{\lambda'},\boldsymbol{\beta}'^{\lambda'})_{S_k}} + \delta_{(\boldsymbol{\alpha}^{\lambda},\boldsymbol{\beta}'^{\lambda'})_{S_k}} \delta_{(\boldsymbol{\alpha}'^{\lambda},\boldsymbol{\beta}^{\lambda'})_{S_k}} \right).$$

Let us define

$$\begin{split} J := & \sum_{\lambda,\lambda'} p_{\lambda} p_{\lambda'} \sum_{\substack{\alpha^{\lambda},\alpha'^{\lambda} \\ \beta^{\lambda'},\beta'^{\lambda'}}} c_{\alpha^{\lambda}} c_{\beta^{\lambda'}}^* c_{\beta'^{\lambda'}}^* \\ & \times \left(\delta_{(\alpha'^{\lambda},\beta^{\lambda'})_{S_h}} \delta_{(\alpha^{\lambda},\beta'^{\lambda'})_{S_h}} - \frac{1}{2^m} \delta_{(\alpha^{\lambda},\alpha'^{\lambda})_{S_h}} \delta_{(\beta^{\lambda'},\beta'^{\lambda'})_{S_h}} \right) \prod_{k \neq h} \left(\delta_{(\alpha^{\lambda},\alpha'^{\lambda})_{S_k}} \delta_{(\beta^{\lambda'},\beta'^{\lambda'})_{S_k}} + \delta_{(\alpha^{\lambda},\beta'^{\lambda'})_{S_k}} \delta_{(\alpha'^{\lambda},\beta^{\lambda'})_{S_k}} \right), \end{split}$$

which, has the form of $J=1-\frac{1}{2^m}+\sum_{l=1}^{2^{\xi-1}-1}\left(\mathcal{A}_l-\frac{1}{2^m}\mathcal{B}_l\right)$, where \mathcal{A}_l , \mathcal{B}_l are the purities of reduced states of ρ . The latter can be understood in the following way. Let us define the set $\mathcal{S}=\{S_1,S_2,\cdots,S_\xi\}$, whose elements represents each block. Then, suppose that we want to consider the partial trace of ρ over several subsystems $\mathcal{H}_{\overline{K}}$, where $\overline{K}\subset\mathcal{S}$. The reduced state lives in the composite Hilbert space \mathcal{H}_K , where $K=\mathcal{S}\setminus\overline{K}$, and we can write $\alpha:=\alpha_K\cdot\alpha_{\overline{K}}$. Let us define the reduced state as $\rho_K:=\mathrm{Tr}_{\overline{K}}[\rho]$, and its purity can be explicitly written as

$$\operatorname{Tr}\left[\rho_{\boldsymbol{K}}^{2}\right] = \sum_{\lambda,\lambda'} p_{\lambda} p_{\lambda'} \sum_{\boldsymbol{\alpha}^{\lambda} \cdot \boldsymbol{\beta}^{\lambda'}} c_{\boldsymbol{\alpha}^{\lambda}} c_{\boldsymbol{\alpha}^{\lambda}}^{*} c_{\boldsymbol{\beta}^{\lambda'}}^{*} c_{\boldsymbol{\beta}^{\lambda'}} c_{\boldsymbol{\alpha}^{\lambda}_{\boldsymbol{K}} \cdot \boldsymbol{\beta}^{\lambda'}_{\boldsymbol{K}}}^{*},$$

which appears in the expression of J. Since Tr $\left[\rho_{\mathbf{K}}^2\right] \leqslant 1$, we have $J < 2^{\xi-1}$; therefor, we can write

$$\operatorname{Var}\left[\partial_{\nu}C_{G}\right] < \frac{2^{2m-2}}{(2^{2m}-1)2^{2m\xi-\xi}(1+2^{-m})^{\xi}} < \frac{1}{2^{\left(2-\frac{1}{m}\right)n}} \quad (\forall m \in \mathbb{N}),$$
(111)

where in the last inequality we used the fact that $n = m\xi$. Equation (111) shows that for the single layer of the alternating layered ansatz the global cost functions presents a barren plateau.

B. Variance of the local cost function partial derivative

Here we consider the case when $V(\theta)$ is given by a single layer of the Alternating Layered Ansatz, and when the local cost function is

$$C_L = 1 - \frac{1}{n} \sum_{j=1}^n \operatorname{Tr} \left[\left(|0\rangle\langle 0|_j \otimes \mathbb{1}_{\overline{j}} \right) V \rho V^{\dagger} \right].$$

with $O_L = \frac{1}{n} \sum_{j=1}^n |0\rangle\langle 0|_j \otimes \mathbb{1}_{\overline{j}}$, and where j denotes the j-th qubit. Moreover, let us assume that we are training a parameter θ_{ν} in h-th block. This case is simpler than the one previously considered for the global cost function as the gradient is non vanishing only when we measure a qubit j in S_h . We can then redefine $O_L^h: \mathcal{H}_h \to \mathcal{H}_h$ as $\widehat{O}_L^h = \frac{1}{n} \sum_{j=1}^m |0\rangle\langle 0|_j \otimes \mathbb{1}_{\overline{j}}$, where each j is such that $j \in S_h$. Then, from (105) we have

$$\operatorname{Tr}\left[\widehat{O}_{L}^{h}\right] = \frac{m2^{m-1}}{n}, \quad \operatorname{Tr}\left[\left(\widehat{O}_{L}^{h}\right)^{2}\right] = \frac{m(m+1)2^{m-2}}{n^{2}}.$$
(112)

From (97), Ω_{qp} can be written as $\Omega_{qp} = \delta_{pq} W_h O_L^h W_h^{\dagger}$, which leads to

$$\Delta\Omega_{pq}^{p'q'} = \frac{m2^{m-2}}{n^2} \delta_{pq} \delta_{p'q'}. \tag{113}$$

Next, from (98) we have $\Psi_{pq} = \text{Tr}_{\overline{h}}[(|q\rangle\langle p|\otimes \mathbb{1}_h)\rho]$, and it is straightforward to see that

$$\sum_{pq} \delta_{pq} \Psi_{pq} = \sum_{pq} \delta_{pq} \operatorname{Tr}_{\overline{h}} \left[(|q\rangle \langle p| \otimes \mathbb{1}_h) \rho \right] = \rho_h, \qquad (114)$$

where we defined $\rho_h := \operatorname{Tr}_{\overline{h}}[\rho]$. Then, from (105), and by using $\left\langle \Delta \Psi_{pq}^{p'q'} \right\rangle_{V_L} = \Delta \Psi_{pq}^{p'q'}$, and $\operatorname{Tr}[\sigma_{\nu}^2] = 2^m$, we can write

$$\operatorname{Var}\left[\partial_{\nu}C_{L}\right] = \frac{m2^{3(m-1)}}{n^{2}(2^{2m}-1)^{2}} \left(\operatorname{Tr}[\rho_{h}^{2}] - \frac{1}{2^{m}}\right) = \frac{m \cdot 2^{3(m-1)}}{n^{2}(2^{2m}-1)^{2}} D_{HS}\left(\rho_{h}, \frac{1}{2^{m}}\right),$$

where $D_{HS}(\rho_h, \mathbb{1}/2^m)$ is the Hilbert-Schmidt distance between ρ_h and $\mathbb{1}/2^m$. If $D_{HS}(\rho_h, \mathbb{1}/2^m) \in \Omega(1/\operatorname{poly}(n))$, we have that the variance of the cost function partial derivative is polinomially vanishing with n as

$$\operatorname{Var}[\partial_{\nu}C_L] \in \Omega\left(\frac{1}{\operatorname{poly}(n)}\right),\tag{115}$$

and hence in this case C_L presents no barren plateau.

Supplementary Note 6: Proof of Theorem 2

First, let us recall that we are considering m-local cost functions where each operator O_i acts nontrivially on m qubits $O_i = \mathbb{1}_{\overline{m}} \otimes \widehat{O}_i$ (here $\mathbb{1}_{\overline{m}}$ indicates the identity on all but m qubits), and where \widehat{O}_i can be expressed as $\widehat{O}_i = \widehat{O}_i^{\mu_i} \otimes \widehat{O}_i^{\mu'_i}$. Hence, we have

$$O = c_0 \mathbb{1} + \sum_{i=1}^{N} c_i \widehat{O}_i^{\mu_i} \otimes \widehat{O}_i^{\mu_i'}, \tag{116}$$

where $\hat{O}_i^{\mu_i}$ are operators acting on m/2 qubits which can be written as tensor product of Pauli operators. Here we recall that we have defined S_k as the m-qubit subsystem on which W_{kL} acts and let $\mathcal{S} = \{S_k\}$ be the set of all such subsystems. As detailed in the main text the summation in Eq. (116) includes two possible cases: First, when $\hat{O}_i^{\mu_i}$ ($\hat{O}_i^{\mu_i'}$) acts on the first (last) m/2 qubits of a given S_k , and second, when $\hat{O}_i^{\mu_i}$ ($\hat{O}_i^{\mu_i'}$) acts on the last (first) m/2 qubits of a given S_k (S_{k+1}). This type of cost function includes any ultralocal (i.e., where the O_i are one-body) cost function, and also VQE Hamiltonians with up to m/2 neighbor interactions.

Here we provide a proof of Theorem 2 in the main text, which we now reiterate for convenience.

Theorem 2. Consider a trainable parameter θ^{ν} in a block W of the ansatz $V(\theta)$. Let $Var[\partial_{\nu}C]$ be the variance of the partial derivative of an m-local cost function C (with O given by (116)) with respect to θ^{ν} . If each block in $V(\theta)$ forms a local 2-design, then $Var[\partial_{\nu}C]$ is lower bounded by

$$G_n(L,l) \leqslant \operatorname{Var}[\partial_{\nu}C],$$
 (117)

with

$$G_n(L,l) = \frac{2^{m(l+1)-1}}{(2^{2m}-1)^2(2^m+1)^{L+l}} \sum_{i \in i_{\mathcal{L}}} \sum_{\substack{(k,k') \in k_{\mathcal{L}_B} \\ k' \geqslant k}} c_i^2 \epsilon(\rho_{k,k'}) \epsilon(\widehat{O}_i), \qquad (118)$$

where $i_{\mathcal{L}}$ is the set of i indices whose associated operators \widehat{O}_i act on qubits in the forward light-cone \mathcal{L} of W, and $k_{\mathcal{L}_B}$ is the set of k indices whose associated subsystems S_k are in the backward light-cone \mathcal{L}_B of W. Here we defined the function $\epsilon(M) = D_{HS}(M, \operatorname{Tr}(M) \mathbb{1}/d_M)$ where D_{HS} is the Hilbert-Schmidt distance and d_M is the dimension of the matrix M. In addition, $\rho_{k,k'}$ is partial trace of the input state ρ down to the subsystems $S_k S_{k+1}...S_{k'}$.

Proof. Let us first consider the case when the operators O_i are of the form (116) and act non trivially in a given subsystem of S. We can expand

$$\operatorname{Var}[\partial_{\nu}C] = \frac{2^{m-1}\operatorname{Tr}[\sigma_{\nu}^{2}]}{(2^{2m}-1)^{2}} \sum_{i,j} \sum_{\substack{pq \ p'q'}} c_{i}c_{j} \left\langle \operatorname{Tr}[\Omega_{qp}^{i}\Omega_{q'p'}^{j}] - \frac{\operatorname{Tr}[\Omega_{qp}^{i}]\operatorname{Tr}[\Omega_{q'p'}^{j}]}{2^{m}} \right\rangle_{V_{R}} \left\langle \Delta\Psi_{pq}^{p'q'} \right\rangle_{V_{L}}, \tag{119}$$

where we defined

$$\Omega_{qp}^{i} = \operatorname{Tr}_{\overline{w}} \left[(|\boldsymbol{p}\rangle\langle \boldsymbol{q}| \otimes \mathbb{1}_{w}) V_{R}^{\dagger} O_{i} V_{R} \right]. \tag{120}$$

We recall here that we assume without loss of generality that V_R contains the gates in \mathcal{L} and all the blocks W_{kL} in the last layer of $V(\theta)$. Hence, we can express

$$V_R = V_{\overline{L}} \otimes V_{\mathcal{L}}, \tag{121}$$

where $V_{\mathcal{L}}$ contains all the blocks in the forward light-cone \mathcal{L} of W, and where $V_{\overline{\mathcal{L}}}$ consists of all the remaining blocks in the last layer of the ansatz. When analyzing the operators Ω^i_{pq} we have to consider two cases: 1) when O_i only acts non-trivially on qubits in $S_{\overline{\mathcal{L}}}$, and 2) when \widehat{O}_i acts non-trivially on qubits in $S_{\mathcal{L}}$. If O_i only acts non-trivially on qubits in $S_{\overline{\mathcal{L}}}$, it is straightforward to show from (120) that $\Omega^i_{pq} \propto \mathbb{1}_w$. Hence, in this case, we find

$$\operatorname{Tr}\left[\Omega_{\boldsymbol{qp}}^{i}\Omega_{\boldsymbol{q'p'}}^{j}\right] - \frac{\operatorname{Tr}\left[\Omega_{\boldsymbol{qp}}^{i}\right]\operatorname{Tr}\left[\Omega_{\boldsymbol{q'p'}}^{j}\right]}{2^{m}} = 0.$$
(122)

Let us then define $i_{\mathcal{L}}$ as the set of i indices whose associated operators O_i act on qubits in the forward light-cone \mathcal{L} of W. In what follows we assume that the indexes $i, j \in i_{\mathcal{L}}$, i.e., we assume that O_i and O_j act non-trivially on qubit in $S_{\mathcal{L}}$. The latter leads to

$$\left\langle \operatorname{Tr}[\Omega_{\boldsymbol{qp}}^{i}\Omega_{\boldsymbol{q'p'}}^{j}] - \frac{\operatorname{Tr}[\Omega_{\boldsymbol{qp}}^{i}]\operatorname{Tr}[\Omega_{\boldsymbol{q'p'}}^{j}]}{2^{m}} \right\rangle_{V_{\mathcal{P}}} = \delta_{(\boldsymbol{p},\boldsymbol{q})_{S_{\overline{\mathcal{L}}}}}\delta_{(\boldsymbol{p'},\boldsymbol{q'})_{S_{\overline{\mathcal{L}}}}} \left\langle \operatorname{Tr}[\Omega_{\boldsymbol{qp}}^{i}\Omega_{\boldsymbol{q'p'}}^{j}] - \frac{\operatorname{Tr}[\Omega_{\boldsymbol{qp}}^{i}]\operatorname{Tr}[\Omega_{\boldsymbol{q'p'}}^{j}]}{2^{m}} \right\rangle_{V_{\mathcal{L}}}.$$
 (123)

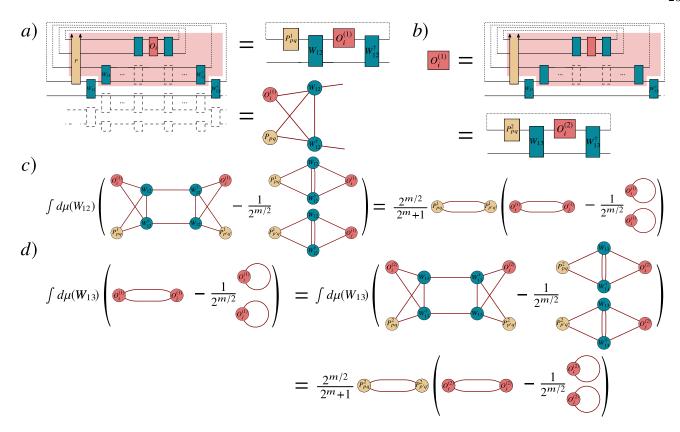
Here the delta functions arise from (120) by noting that $V_R^{\dagger}O_iV_R = V_{\mathcal{L}}^{\dagger}O_iV_{\mathcal{L}}$.

In order to explicitly evaluate the expectation value in (123) we use the fact that each block in the layered ansatz is a 2-design, and hence one can algorithmically integrate over each block using the Weingarten calculus. Specifically, as discussed in the main text we employ the tensor network representation of $\text{Tr}[\Omega^i_{qp}\Omega^i_{q'p'}]$ and $\text{Tr}[\Omega^j_{qp}]\text{Tr}[\Omega^j_{q'p'}]$, and we use the *Random Tensor Network Integrator* (RTNI) package of Ref. [44], which allows for the computation of averages of tensor networks containing multiple Haar-distributed random unitary matrices and deterministic symbolic tensors.

Using this procedure, $\langle \dots \rangle_{V_{\mathcal{L}}}$ can be computed by integrating over each block inside of $V_{\mathcal{L}}$ over the unitary group with the respect to the Haar measure. After each integration the result of the average is a sum of up to four new tensor networks according to (51), and Lemmas 2 and 3. After all the blocks in $V_{\mathcal{L}}$ have been integrated, the final result can be expressed as

$$\left\langle \operatorname{Tr}\left[\Omega_{\boldsymbol{q}\boldsymbol{p}}^{i}\Omega_{\boldsymbol{q'}\boldsymbol{p'}}^{j}\right] - \frac{\operatorname{Tr}\left[\Omega_{\boldsymbol{q}\boldsymbol{p}}^{i}\right]\operatorname{Tr}\left[\Omega_{\boldsymbol{q'}\boldsymbol{p'}}^{j}\right]}{2^{m}}\right\rangle_{V_{\mathcal{C}}} = \sum_{\tau} t_{\tau}^{ij}\delta_{(\boldsymbol{p},\boldsymbol{q})_{S_{\overline{\tau}}}}\delta_{(\boldsymbol{p'},\boldsymbol{q'})_{S_{\overline{\tau}}}}\delta_{(\boldsymbol{p},\boldsymbol{q'})_{S_{\tau}}}\delta_{(\boldsymbol{p'},\boldsymbol{q'})_{S_{\tau}}}\delta_{(\boldsymbol{p'},\boldsymbol{q'})_{S_{\tau}}}\Delta O_{\tau}^{ij},$$

$$(124)$$



SUP FIG. 1. Schematic representation of the method employed to derive Eq. (124). Here we consider the case when O_i and O_j act nontrivially only on the topomost m qubits in $V_{\mathcal{L}}$. (a) Tensor-network representation of the term Ω^i_{qp} . All but L-l blocks in $V_{\mathcal{L}}$ simplify to identity when computing $V_{\mathcal{L}}^{\dagger}O_iV_{\mathcal{L}}$. One can always define operators $O_i^{(1)}$, and $O_j^{(1)}$ such that Eq. (126) holds. Here W_{12} is the topmost block in the first layer of $V_{\mathcal{L}}$, and we define P_{pq}^1 as a projector operator acing on m/2 qubits. (b) Tensor-network representation of the operator $O_i^{(1)}$. Note that from $O_i^{(1)}$ we can also define an operator $O_i^{(2)}$ which will be of the same form as $O_i^{(1)}$. (c) By means of the Weingarten calculus we can integrate over W_{12} to compute the expectation value of Eq. (126). The result is a single tensor. This result can be obtained by employing Eq. (71) of Lemma 6. (d) In order the integrate the next block we use the operators $O_i^{(2)}$ to express the tensor networks in a form that coincides with panel (c). We can then repeat this procedure L-l times in order to integrate over all blocks and compute the expectation value in (123). The final result is of the form of Eq. (127).

where $t_{\tau} \in \mathbb{R}$, $S_{\tau} \cup S_{\overline{\tau}} = S_{\mathcal{L}} \cap S_{\overline{w}}$ (with $S_{\tau} \neq \emptyset$), and where we have defined

$$\Delta O_{\tau}^{ij} = \operatorname{Tr}_{x_{\tau}y_{\tau}} \left[\operatorname{Tr}_{z_{\tau}} \left[O_{i} \right] \operatorname{Tr}_{z_{\tau}} \left[O_{j} \right] \right] - \frac{\operatorname{Tr}_{x_{\tau}} \left[\operatorname{Tr}_{y_{\tau}z_{\tau}} \left[O_{i} \right] \operatorname{Tr}_{y_{\tau}z_{\tau}} \left[O_{j} \right] \right]}{2m} \,. \tag{125}$$

Here we use the notation $\operatorname{Tr}_{x_{\tau}}$ to indicate the trace over the Hilbert space associated with subsystem $S_{x_{\tau}}$. We also define $\mathcal{S}^{\mathcal{L}} = \{S_k : S_k \subset S_{\mathcal{L}}\}$ as the set of subspaces S_k which belong to the light-cone \mathcal{L} , so that we have $S_{y_{\tau}} \in \mathcal{S}^{\mathcal{L}}$, $S_{x_{\tau}} \cup S_{y_{\tau}} \cup S_{z_{\tau}} = S_{\mathcal{L}}$, and $S_{x_{\tau}}, S_{z_{\tau}} \in \mathcal{P}(\mathcal{S}^{\mathcal{L}})$, with $\mathcal{P}(\mathcal{S}^{\mathcal{L}}) = \{\emptyset, S_1, \dots, S_{\xi}, S_1 \cup S_2 \dots\}$ the power set of $\mathcal{S}^{\mathcal{L}}$. If one chooses $S_{z_{\tau}} = \emptyset$ (or $S_{x_{\tau}} = \emptyset$), with associated Hilbert space $H_0 = \{\mathbf{0}\}$, we define $\operatorname{Tr}_{\emptyset}[O] := O$.

Equation (124) can be derived by iteratively applying Lemma 6 each time a block in $V_{\mathcal{L}}$ is integrated in (123), and noting that at each integration the resulting tensor can always be written in a way such that Lemma 6 can be applied again. As an example, let us consider the case when O_i and O_j act nontrivially only on the topomost m qubits in $V_{\mathcal{L}}$. As shown in Fig. 1(a), all but L-l blocks in $V_{\mathcal{L}}$ simplify to identity when computing $V_{\mathcal{L}}^{\dagger}O_iV_{\mathcal{L}}$. Then, let us denote by W_{12} the topmost gate in the first layer in $V_{\mathcal{L}}$, and let \widetilde{S}_1 , \widetilde{S}_2 be the sets of m/2 adjacent qubits (with associated Hilbert spaces $\widetilde{\mathcal{H}}_1$, $\widetilde{\mathcal{H}}_2$) such that W_{12} acts on $\widetilde{\mathcal{H}}_1 \otimes \widetilde{\mathcal{H}}_2$, and such that $\widetilde{S}_2 \subset S_w$. One can always write

$$\left\langle \operatorname{Tr}\left[\Omega_{\boldsymbol{qp}}^{i}\Omega_{\boldsymbol{q'p'}}^{j}\right] - \frac{\operatorname{Tr}\left[\Omega_{\boldsymbol{qp}}^{i}\right]\operatorname{Tr}\left[\Omega_{\boldsymbol{q'p'}}^{j}\right]}{2^{m}}\right\rangle_{V_{\mathcal{L}}} \propto \left\langle \operatorname{Tr}_{\widetilde{\mathcal{H}}_{2}}\left[\operatorname{Tr}_{\widetilde{\mathcal{H}}_{1}}[\Omega_{1}]\operatorname{Tr}_{\widetilde{\mathcal{H}}_{1}}[\Omega'_{1}]\right] - \frac{\operatorname{Tr}\left[\Omega_{1}\right]\operatorname{Tr}\left[\Omega'_{1}\right]}{2^{m}}\right\rangle_{V_{\mathcal{L}}},$$
(126)

with $\Omega_1 = W_{12}O_i^{(1)}W_{12}^{\dagger}(|\boldsymbol{p}\rangle\langle\boldsymbol{q}|_{\widetilde{S}_1}\otimes\mathbb{1}_{\widetilde{S}_2}),\ \Omega_1' = W_{12}O_j^{(1)}W_{12}^{\dagger}(|\boldsymbol{p}'\rangle\langle\boldsymbol{q}'|_{\widetilde{S}_1}\otimes\mathbb{1}_{\widetilde{S}_2}),\ \text{and where }O_i^{(1)},\ \text{and }O_j^{(1)}\ \text{are defined}$

according to Fig. 1(a). The proportionallity factor in Eq. (126) is given by delta functions over p, and q. Moreover, the right-hand side of (126) is exactly of the form (64), and hence by applying Lemma 6 (or more specifically, Eq. (71)) one finds the result of Fig. 1(c). As schematically depicted in Fig. 1(b), one can then define operators $O_i^{(2)}$ and repeat this calculation L-l times as in Fig. 1(d). One finally finds

$$\left\langle \operatorname{Tr}\left[\Omega_{\boldsymbol{qp}}^{i}\Omega_{\boldsymbol{q'p'}}^{j}\right] - \frac{\operatorname{Tr}\left[\Omega_{\boldsymbol{qp}}^{i}\right]\operatorname{Tr}\left[\Omega_{\boldsymbol{q'p'}}^{j}\right]}{2^{m}}\right\rangle_{V_{\mathcal{L}}} \propto \frac{2^{m(L-l)/2}}{(2^{m}+1)^{L-l}} \left(\operatorname{Tr}\left[O_{i}O_{j}\right] - \frac{\operatorname{Tr}\left[O_{i}\right]\operatorname{Tr}\left[O_{j}\right]}{2^{m}}\right), \tag{127}$$

where once again the proportionally factor is given by delta functions over p and q. For more general operators O_i and O_j , each time a block is integrated, one can always rewrite the resulting non-trivial terms in the form of either Eq. (64), or Eq. (68). Remarkably, this means that the final result can always be expressed in terms of contractions of the form (125), and hence Eq. (124) holds.

As previously mentioned, Eq. (124) is valid for arbitrary operators O_i and O_j . However, from Lemma 7 we know that if O_i and O_j have no overlapping support, then $\Delta O_{\tau}^{ij} = 0$, for all τ . Hence we only have to consider the cases when i = j. Moreover, if \hat{O}_i act non trivially in a given subsystem of \mathcal{S} the summation in Eq. (124) simplifies and we find

$$\left\langle \operatorname{Tr}\left[\Omega_{\boldsymbol{q}\boldsymbol{p}}^{i}\Omega_{\boldsymbol{q}'\boldsymbol{p}'}^{j}\right] - \frac{\operatorname{Tr}\left[\Omega_{\boldsymbol{q}\boldsymbol{p}}^{i}\right]\operatorname{Tr}\left[\Omega_{\boldsymbol{q}'\boldsymbol{p}'}^{j}\right]}{2^{m}}\right\rangle_{V_{\mathcal{L}}} = \epsilon(\widehat{O}_{i})\sum_{\tau}\hat{t}_{\tau}^{ii}\delta_{(\boldsymbol{p},\boldsymbol{q})_{S_{\tau}}}\delta_{(\boldsymbol{p}',\boldsymbol{q}')_{S_{\tau}}}\delta_{(\boldsymbol{p},\boldsymbol{q}')_{S_{\tau}}}\delta_{(\boldsymbol{p}',\boldsymbol{q}')_{S_{\tau}}},$$
(128)

where we now denote the coefficients as \hat{t}_{τ}^{ii} since we now have $\hat{t}_{\tau}^{ii} \geq 0$, and where

$$\epsilon(\widehat{O}_i) = \operatorname{Tr}\left[\widehat{O}_i^2\right] - \frac{\operatorname{Tr}\left[\widehat{O}_i\right]^2}{2^m} = D_{HS}\left(\widehat{O}_i, \operatorname{Tr}[\widehat{O}_i] \frac{1}{2^m}\right). \tag{129}$$

Moreover, we also find that the following inequality holds $\forall i$

$$\sum_{\tau} \hat{t}_{\tau}^{ii} \geqslant \frac{2^{m(L-l)/2}}{(2^m+1)^{L-l}},\tag{130}$$

where we recall that L is the number of layers in the ansatz, and that the block W is in the lth-layer of $V(\theta)$. This result can be understood from (127) by noting that when O_i does not act on the topmost qubits of $V_{\mathcal{L}}$ there are more terms that will contribute to the summation over τ in (130), and hence the bound holds. Combining Eqs. (119) and (128), we find

$$\operatorname{Var}[\partial_{\nu}C] = \frac{2^{m-1}\operatorname{Tr}[\sigma_{\nu}^{2}]}{(2^{2m}-1)^{2}} \sum_{\substack{\boldsymbol{p}\boldsymbol{q} \\ \boldsymbol{p}'\boldsymbol{q}'}} \sum_{i \in i_{\mathcal{L}}} c_{i}^{2} \epsilon(\widehat{O}_{i}) \sum_{\tau} \hat{t}_{\tau}^{ii} \delta_{(\boldsymbol{p},\boldsymbol{q})_{S_{\overline{\mathcal{L}}} \cup S_{\overline{\tau}}}} \delta_{(\boldsymbol{p}',\boldsymbol{q}')_{S_{\overline{\tau}}} \cup S_{\overline{\tau}}} \delta_{(\boldsymbol{p},\boldsymbol{q}')_{S_{\tau}}} \delta_{(\boldsymbol{p}',\boldsymbol{q}')_{S_{\tau}}} \left\langle \Delta \Psi_{\boldsymbol{p}\boldsymbol{q}}^{\boldsymbol{p}'\boldsymbol{q}'} \right\rangle_{V_{L}}. \tag{131}$$

Let us now consider the term

$$\left\langle \Delta \Psi_{pq}^{p'q'} \right\rangle_{V_L} = \left\langle \text{Tr}[\Psi_{pq}\Psi_{p'q'}] - \frac{\text{Tr}[\Psi_{pq}]\text{Tr}[\Psi_{p'q'}]}{2^m} \right\rangle_{V_L}. \tag{132}$$

Since the bitstring p(q) can be expressed as a bit-wise concatenation of the form $p = (p)_{S_{\overline{L}} \cup S_{\overline{\tau}}} \cdot (p)_{S_{\tau}}$ (and similarly for q), then we can first evaluate

$$\sum_{(\boldsymbol{p}\boldsymbol{q})_{S_{\mathcal{T}}\cup S_{\mathcal{T}}}} \delta_{(\boldsymbol{p},\boldsymbol{q})_{S_{\mathcal{T}}\cup S_{\mathcal{T}}}} \Psi_{\boldsymbol{q}\boldsymbol{p}} = \operatorname{Tr}_{\tau} \left[(|\boldsymbol{p}\rangle\langle \boldsymbol{q}|_{S_{\tau}} \otimes \mathbb{1}_{w}) \tilde{\rho}_{Wk} \right], \qquad (133)$$

where Tr_{τ} is the partial trace over the Hilbert space \mathcal{H}_{τ} of the qubits in S_{τ} , and where we defined

$$\tilde{\rho}_{Wk} = \text{Tr}_{\overline{\mathcal{L}} \cup \overline{\tau}} [V_L \rho V_L^{\dagger}], \qquad (134)$$

as the reduced state of $V_L \rho V_L^{\dagger}$ on $\mathcal{H}_w \otimes \mathcal{H}_{\tau}$. Then, from the term $\delta_{(\boldsymbol{p},\boldsymbol{q}')_{S_{\tau}}} \delta_{(\boldsymbol{p}',\boldsymbol{q})_{S_{\tau}}}$ in (131), we get

$$\sum_{(\boldsymbol{p}\boldsymbol{q})_{S_{\tau}}} \delta_{(\boldsymbol{p},\boldsymbol{q}')_{S_{\tau}}} \delta_{(\boldsymbol{p}',\boldsymbol{q})_{S_{\tau}}} \left(\operatorname{Tr}[\Psi_{\boldsymbol{p}\boldsymbol{q}}\Psi_{\boldsymbol{q}\boldsymbol{p}}] - \frac{\operatorname{Tr}[\Psi_{\boldsymbol{p}\boldsymbol{q}}]\operatorname{Tr}[\Psi_{\boldsymbol{q}\boldsymbol{p}}]}{2^{m}} \right) = D_{HS} \left(\tilde{\rho}_{w\tau}, \tilde{\rho}_{\tau} \otimes \frac{1}{2^{m}} \right), \tag{135}$$

where we defined

$$\tilde{\rho}_{\tau} = \operatorname{Tr}_{w}(\tilde{\rho}_{w\tau}), \quad \text{and} \quad \tilde{\rho}_{w} = \operatorname{Tr}_{\tau}(\tilde{\rho}_{w\tau}) = \operatorname{Tr}_{\overline{w}}\left[V_{L}\rho V_{L}^{\dagger}\right],$$
(136)

as the reduces states of $V_L \rho V_L^{\dagger}$ on subsystem \mathcal{H}_{τ} , and \mathcal{H}_w , respectively. Equation (135) quantifies how far $\tilde{\rho}_{w\tau}$ is from being a tensor product state where the state on subsystem S_w is maximally mixed. Evidently, if $\tilde{\rho}_w$ is maximally mixed then it will be impossible to train any angle in W.

Let us now analyze the following chain of inequalities valid for any Hilbert-Schmidt distance $D_{HS}\left(\tilde{\rho}_{w\tau_t}, \tilde{\rho}_{\tau_t} \otimes \frac{1}{2^m}\right)$ and any choice of S_{τ} :

$$D_{HS}\left(\tilde{\rho}_{w\tau_{t}}, \tilde{\rho}_{\tau_{t}} \otimes \frac{1}{2^{m}}\right) \geqslant \frac{4D_{T}\left(\tilde{\rho}_{w\tau_{t}}, \tilde{\rho}_{\tau_{t}} \otimes \frac{1}{2^{m}}\right)^{2}}{2^{m}d_{\tau}}$$

$$\geqslant \frac{4D_{T}\left(\tilde{\rho}_{w}, \frac{1}{2^{m}}\right)^{2}}{2^{m(L-l+2)/2}}$$

$$\geqslant \frac{D_{HS}\left(\tilde{\rho}_{w}, \frac{1}{2^{m}}\right)}{2^{m(L-l+2)/2}},$$
(138)

with $D_T(A, B) = \text{Tr}\left[\sqrt{(A-B)^2}\right]$ the Trace Distance between the Hermitian operators A and B. In the first line we employ the matrix norm equivalence, and we denote as d_{τ} the dimension of \mathcal{H}_{τ} . The second line is derived from the fact that the Trace Distance is non-increasing over partial trace [45], and from the fact that $d_{\tau} \leq 2^{m(L-l)/2} \, \forall \tau$. Finally, the inequality in (138) employs again the matrix norm equivalence. From Eqs. (138), and (131), we find that the following lower bound holds

$$\operatorname{Var}[\partial_{\nu}C] \geqslant \frac{\operatorname{Tr}[\sigma_{\nu}^{2}]}{2(2^{2m}-1)^{2}(2^{m}+1)^{L-l}} \sum_{i \in i_{C}} c_{i}^{2} \epsilon_{i} \left\langle D_{HS}\left(\widetilde{\rho}_{w}, \frac{1}{2^{m}}\right) \right\rangle_{V_{L}}.$$
(139)

Following a similar procedure as the one previously employed to compute expectation values over V_R , we can once again leverage the tensor network representation of quantum circuits to algorithmically integrate over each block and compute $\langle D_{HS}\left(\tilde{\rho}_W,\frac{1}{2^m}\right)\rangle_{V_L}$. After considering that all the blocks in V_L which are not in the backpropagated light-cone of W will simplify to identity, we find

$$\left\langle D_{HS}\left(\tilde{\rho}_{w}, \frac{1}{2^{m}}\right)\right\rangle_{V_{L}} = \sum_{\substack{(k,k')\in k_{\mathcal{L}_{B}}\\k'\geqslant k}} t_{k,k'} \epsilon(\rho_{k,k'}), \qquad (140)$$

where $t_{k,k'} \ge 0$, and where $k_{\mathcal{L}_B}$ is the set of k indices whose associated subsystems S_k are in the backward light-cone \mathcal{L}_B of W. Here we defined the function $\epsilon(M) = D_{\mathrm{HS}}\left(M, \mathrm{Tr}(M)\mathbb{1}/d_M\right)$ where D_{HS} is the Hilbert-Schmidt distance and d_M is the dimension of the matrix M. In addition, $\rho_{k,k'}$ is partial trace of the input state ρ down to the subsystems $S_k S_{k+1}...S_{k'}$. In addition, we find that the following inequality holds $\forall k,k'$

$$t_{k,k'} \geqslant \frac{2^{ml}}{(2^m + 1)^{2l}}. (141)$$

Hence, we have $\operatorname{Var}[\partial_{\nu}C] \geqslant G_n(L,l)$, where

$$G_n(L,l) = \frac{2^{m(l+1)-1}}{(2^{2m}-1)^2(2^m+1)^{L+l}} \sum_{i \in i_{\mathcal{L}}} \sum_{\substack{(k,k') \in k_{\mathcal{L}_B} \\ k' > k}} c_i^2 \epsilon(\rho_{k,k'}) \epsilon(\widehat{O}_i), \qquad (142)$$

where we used the fact that $Tr[\sigma_{\nu}^2] = 2^m$.

This result can be trivially generalized to the case when \hat{O}_i and \hat{O}_j are of the general form in Eq. (116) such that they can have overlapping support on at most m/2 qubits. Then, from (125) it is straightforward to see that $\Delta O_{\tau}^{ij} = 0$ for all τ , i, and j, as one would always have to compute traces of the form $\text{Tr}[\hat{O}_i^{\mu_i}]$, which vanish since $\hat{O}_i^{\mu_i}$ can be written as a tensor product of Pauli operators.

Supplementary Note 7: Proof of Theorem 1

The following theorem provides an upper bound on the variance of the partial derivative of a global cost function which can be expressed as the expectation value of an operator of the form

$$O = c_0 \mathbb{1} + \sum_{i=1}^{N} c_i \hat{O}_{i1} \otimes \hat{O}_{i2} \otimes \cdots \otimes \hat{O}_{i\xi}.$$

$$(143)$$

Specifically, we consider two cases of interest: (i) When N=1 and each \widehat{O}_{1k} is a non-trivial projector $(\widehat{O}_{1k}^2 = \widehat{O}_{1k} \neq 1)$ of rank r_k acting on subsystem S_k , or (ii) When N is arbitrary and \widehat{O}_{ik} is traceless with $\text{Tr}[\widehat{O}_{ik}^2] \leq 2^m$ (for example, when $\widehat{O}_{ik} = \bigotimes_{j=1}^m \sigma_j^{\mu}$ is a tensor product of Pauli operators $\sigma_j^{\mu} \in \{1, \sigma_j^x, \sigma_j^y, \sigma_j^z\}$, with at least one $\sigma_j^{\mu} \neq 1$). In Section 7 A we first consider case (i), while in Section 7 B we prove Theorem 1 for case (ii).

We now reiterate Theorem 1 for convenience:

Theorem 1. Consider a trainable parameter θ^{ν} in a block W of the ansatz $V(\theta)$. Let $Var[\partial_{\nu}C]$ be the variance of the partial derivative of a global cost function C (with O given by (143)) with respect to θ^{ν} . If each block in $V(\theta)$ forms a local 2-design, then $Var[\partial_{\nu}C]$ is upper bounded by

$$Var[\partial_{\nu}C] \leqslant F_n(L,l). \tag{144}$$

(i) For N=1 and when each \widehat{O}_{1k} is a non-trivial projector, then defining $R=\prod_{k=1}^{\xi}r_k^2$, we have

$$F_n(L,l) = \frac{2^{2m + (2m-1)(L-l)}}{(2^{2m} - 1) \cdot 3^{\frac{n}{m}} \cdot 2^{(2-\frac{3}{m})n}} c_1^2 R.$$
(145)

(ii) For arbitrary N and when each \hat{O}_{ik} satisfies $\text{Tr}[\hat{O}_{ik}] = 0$ and $\text{Tr}[\hat{O}_{ik}^2] \leqslant 2^m$, then

$$F_n(L,l) = \frac{2^{2m(L-l+1)+1}}{3^{\frac{2n}{m}} \cdot 2^{(3-\frac{4}{m})n}} \sum_{i,j=1}^{N} c_i c_j.$$
(146)

A. N=1, and \widehat{O}_{1k} is a non-trivial projector

For simplicity, let us now use \widehat{O}_k when referring to the operators \widehat{O}_{ik} . Let us first consider the case when each \widehat{O}_k is a non-trivial projector $(\widehat{O}_k^2 = \widehat{O}_k)$ of rank r_k acting on subsystem S_k :

$$r_k := \operatorname{Tr}\left[\widehat{O}_k\right] = \operatorname{Tr}\left[\widehat{O}_k^2\right] = \operatorname{rank}\left[\widehat{O}_k\right].$$
 (147)

Proof. In the previous section, we defined V_R as containing all gates in the forward light-cone $\mathcal L$ of W and all the gates in the last layer of the ansatz. Hence, we can express $V_R = V_{\mathcal L} \otimes V_{\overline{\mathcal L}}$, where $V_{\overline{\mathcal L}} : \mathcal H_{\overline{\mathcal L}} \to \mathcal H_{\overline{\mathcal L}}$ is given by

$$V_{\overline{\mathcal{L}}} = \bigotimes_{k \in k_{\overline{\mathcal{L}}}} W_{kL} \,, \tag{148}$$

where where $k_{\overline{L}}$ is the set of k indices whose associated subsystems of qubits S_k are outside of the forward light-cone \mathcal{L} of W. One can always write $|q\rangle\langle p|\otimes \mathbb{1}_w$ as a projector onto $H_{\mathcal{L}}$ times a projector onto $H_{\overline{L}}$:

$$|\mathbf{q}\rangle\langle\mathbf{p}|\otimes\mathbb{1}_w = \left(\bigotimes_{k\in k_{\overline{\mathcal{L}}}} |\mathbf{q}\rangle\langle\mathbf{p}|_k\right)\otimes|\mathbf{q}\rangle\langle\mathbf{p}|_{\mathcal{L}}\otimes\mathbb{1}_w.$$
 (149)

Combining (97) with Eqs. (148) and (149) leads to

$$\Omega_{qp} = \left(\prod_{k \in k_{\overline{L}}} \operatorname{Tr}_{k} \left[| \boldsymbol{p} \rangle \langle \boldsymbol{q} |_{k} W_{kL}^{\dagger} \widehat{O}_{k} W_{kL} \right] \right) \Omega_{qp}^{\mathcal{L}}, \tag{150}$$

where

$$\Omega_{qp}^{\mathcal{L}} = \operatorname{Tr}_{\mathcal{L} \cap \overline{w}} \left[(|p\rangle \langle q| \otimes \mathbb{1}_w) V_{\mathcal{L}} O^{\mathcal{L}} V_{\mathcal{L}} \right] , \tag{151}$$

and where $O^{\mathcal{L}} = \bigotimes_{k \in k_{\overline{\mathcal{L}}}} \widehat{O}_k$. Here Tr_k indicates the trace over \mathcal{H}_k , while $\operatorname{Tr}_{\mathcal{L} \cap \overline{w}}$ is the trace over the Hilbert space associated with the qubits in $S_{\mathcal{L}} \cap S_{\overline{w}}$.

In order to explicitly evaluate the expectation value $\langle \dots \rangle_{V_R}$ in

$$\operatorname{Var}[\partial_{\nu}C] = \frac{2^{m-1}\operatorname{Tr}[\sigma_{\nu}^{2}]}{(2^{2m}-1)^{2}}c_{1}^{2}\sum_{\substack{pq\\p'q'}}\left\langle \left(\operatorname{Tr}[\Omega_{qp}\Omega_{q'p'}] - \frac{\operatorname{Tr}[\Omega_{qp}]\operatorname{Tr}[\Omega_{q'p'}]}{2^{m}}\right)\right\rangle_{V_{R}}\left\langle \Delta\Psi_{pq}^{p'q'}\right\rangle_{V_{L}},\tag{152}$$

we use the fact that the blocks in $V(\theta)$ are independent, and hence $\langle \dots \rangle_{V_R} = \langle \dots \rangle_{V_{\overline{C}}, V_{\mathcal{L}}}$. Then, we have

$$\left\langle \operatorname{Tr}[\Omega_{\boldsymbol{qp}}\Omega_{\boldsymbol{q'p'}}] - \frac{\operatorname{Tr}[\Omega_{\boldsymbol{qp}}]\operatorname{Tr}[\Omega_{\boldsymbol{q'p'}}]}{2^m} \right\rangle_{V_R} = \left\langle \operatorname{Tr}[\Omega_{\boldsymbol{qp}}^{\mathcal{L}}\Omega_{\boldsymbol{q'p'}}^{\mathcal{L}}] - \frac{\operatorname{Tr}[\Omega_{\boldsymbol{qp}}^{\mathcal{L}}]\operatorname{Tr}[\Omega_{\boldsymbol{q'p'}}^{\mathcal{L}}]}{2^m} \right\rangle_{V_{\mathcal{L}}} \left(\prod_{k/S_k \subset S_{\overline{\mathcal{L}}}} \langle \Omega_k \rangle_{W_{kL}} \right), \quad (153)$$

with

$$\Omega_k = \operatorname{Tr}_k \left[|\boldsymbol{p}\rangle\langle \boldsymbol{q}|_k W_{kL}^{\dagger} \widehat{O}_k W_{kL} \right] \operatorname{Tr}_k \left[|\boldsymbol{p}'\rangle\langle \boldsymbol{q}'|_k W_{kL}^{\dagger} \widehat{O}_k W_{kL} \right]. \tag{154}$$

Let us first compute the expectation value of each Ω_k . From Lemma 3, we have:

$$\langle \Omega_k \rangle_{W_{kL}} = \frac{r_k}{2^{2m} - 1} \left(\left(r_k - \frac{1}{2^m} \right) \delta_{(\boldsymbol{p}, \boldsymbol{q})_{S_k}} \delta_{(\boldsymbol{p}', \boldsymbol{q}')_{S_k}} + \left(1 - \frac{r_k}{2^m} \right) \delta_{(\boldsymbol{p}, \boldsymbol{q}')_{S_k}} \delta_{(\boldsymbol{p}', \boldsymbol{q})_{S_k}} \right)$$

$$\leq \frac{1}{2^{2m} - 1} r_k^2 \left(\delta_{(\boldsymbol{p}, \boldsymbol{q})_{S_k}} \delta_{(\boldsymbol{p}', \boldsymbol{q}')_{S_k}} + \delta_{(\boldsymbol{p}, \boldsymbol{q}')_{S_k}} \delta_{(\boldsymbol{p}', \boldsymbol{q})_{S_k}} \right),$$

$$(155)$$

where in the inequality we have dropped the negative terms and used the fact that $r_k \leqslant r_k^2$. Then, we have

$$\prod_{k \in k_{\overline{L}}} \langle \Omega_k \rangle_{W_{kL}} \leqslant \frac{1}{(2^{2m} - 1)^{\xi_{\overline{L}}}} \prod_{k \in k_{\overline{L}}} r_k^2 \left(\delta_{(\boldsymbol{p}, \boldsymbol{q})_{S_k}} \delta_{(\boldsymbol{p}', \boldsymbol{q}')_{S_k}} + \delta_{(\boldsymbol{p}, \boldsymbol{q}')_{S_k}} \delta_{(\boldsymbol{p}', \boldsymbol{q})_{S_k}} \right).$$

Combining this result with Eq. (152) leads to the upper bound

$$\operatorname{Var}[\partial_{\nu}C] \leqslant \frac{2^{m-1}\operatorname{Tr}[\sigma_{\nu}^{2}]}{(2^{2m}-1)^{2}(2^{2m}-1)^{\xi_{\overline{L}}}}c_{1}^{2}\sum_{\boldsymbol{p}\boldsymbol{q}}\left(\left\langle\operatorname{Tr}[\Omega_{\boldsymbol{q}\boldsymbol{p}}^{\mathcal{L}}\Omega_{\boldsymbol{q'}\boldsymbol{p'}}^{\mathcal{L}}] - \frac{\operatorname{Tr}[\Omega_{\boldsymbol{q}\boldsymbol{p}}^{\mathcal{L}}]\operatorname{Tr}[\Omega_{\boldsymbol{q'}\boldsymbol{p'}}^{\mathcal{L}}]}{2^{m}}\right\rangle_{V_{\mathcal{L}}}\right) \times \left(\prod_{k\in k_{\overline{L}}}r_{k}^{2}\left(\delta_{(\boldsymbol{p},\boldsymbol{q})_{S_{k}}}\delta_{(\boldsymbol{p'},\boldsymbol{q'})_{S_{k}}} + \delta_{(\boldsymbol{p},\boldsymbol{q'})_{S_{k}}}\delta_{(\boldsymbol{p'},\boldsymbol{q})_{S_{k}}}\right)\right)\left\langle\Delta\Psi_{\boldsymbol{p}\boldsymbol{q'}}^{\boldsymbol{p'}\boldsymbol{q'}}\right\rangle_{V_{L}}\right).$$

$$(156)$$

As discussed in the previous section, one can compute the expectation values in Eq. (156) by systematically integrating over each block over the unitary group with the respect to the Haar measure. From Eq. (124) we can find

$$\operatorname{Var}[\partial_{\nu}C] \leq \frac{2^{m-1}\operatorname{Tr}[\sigma_{\nu}^{2}]}{(2^{2m}-1)^{2}(2^{2m}-1)^{\xi_{\overline{L}}}} c_{1}^{2} \sum_{\substack{pq \ p'q'}} \sum_{\tau} \left(t_{\tau} \delta_{(p,q)_{S_{\overline{\tau}}}} \delta_{(p',q')_{S_{\overline{\tau}}}} \delta_{(p,q')_{S_{\tau}}} \delta_{(p',q)_{S_{\tau}}} \Delta O_{\tau} \right) \times \left(\prod_{k \in k_{\overline{L}}} r_{k}^{2} \left(\delta_{(p,q)_{S_{k}}} \delta_{(p',q')_{S_{k}}} + \delta_{(p,q')_{S_{k}}} \delta_{(p',q)_{S_{k}}} \right) \left\langle \Delta \Psi_{pq}^{p'q'} \right\rangle_{V_{L}} \right).$$

$$(157)$$

Note that by expanding the product $\prod_{k \in k_{\overline{L}}} \left(\delta_{(\boldsymbol{p},\boldsymbol{q})_{S_k}} \delta_{(\boldsymbol{p}',\boldsymbol{q}')_{S_k}} + \delta_{(\boldsymbol{p},\boldsymbol{q}')_{S_k}} \delta_{(\boldsymbol{p}',\boldsymbol{q})_{S_k}} \right) \delta_{(\boldsymbol{p},\boldsymbol{q})_{S_{\overline{\tau}}}} \delta_{(\boldsymbol{p}',\boldsymbol{q}')_{S_{\overline{\tau}}}} \delta_{(\boldsymbol{p}',\boldsymbol{q}')_{S_{\tau}}} \delta_{(\boldsymbol{p}',\boldsymbol{q}')$

$$\sum_{\substack{\boldsymbol{p}\boldsymbol{q}\\\boldsymbol{p'}\boldsymbol{q'}}} \delta_{(\boldsymbol{p},\boldsymbol{q})_{S_{\overline{\tau}}}} \delta_{(\boldsymbol{p'},\boldsymbol{q'})_{S_{\overline{\tau}}}} \delta_{(\boldsymbol{p},\boldsymbol{q'})_{S_{\tau}}} \delta_{(\boldsymbol{p'},\boldsymbol{q})_{S_{\tau}}} \left(\prod_{k \in k_{\overline{L}}} \left(\delta_{(\boldsymbol{p},\boldsymbol{q})_{S_{k}}} \delta_{(\boldsymbol{p'},\boldsymbol{q'})_{S_{k}}} + \delta_{(\boldsymbol{p},\boldsymbol{q'})_{S_{k}}} \delta_{(\boldsymbol{p'},\boldsymbol{q})_{S_{k}}} \right) \right) \left\langle \Delta \Psi_{\boldsymbol{p}\boldsymbol{q}}^{\boldsymbol{p'}\boldsymbol{q'}} \right\rangle_{V_{L}} \leqslant 2 \cdot 2^{\xi_{\overline{L}}}. \quad (158)$$

Replacing this result in (157) leads to

$$\operatorname{Var}[\partial_{\nu}C] \leqslant \frac{2^{m}2^{\xi_{\overline{L}}}\operatorname{Tr}[\sigma_{\nu}^{2}]}{(2^{m}-1)^{2}(2^{2m}-1)^{\xi_{\overline{L}}}}c_{1}^{2}\left(\prod_{k\in k_{\overline{L}}}r_{k}^{2}\right)\sum_{\tau}t_{\tau}\Delta O_{\tau}.$$
(159)

Next, we consider the terms ΔO_{τ} . From Eq. (125) we can show that

$$\Delta O_{\tau} \leqslant \prod_{k \in k_C} r_k^2 \,, \tag{160}$$

so that (159) becomes

$$\operatorname{Var}[\partial_{\nu}C] \leqslant \frac{2^{m} 2^{\xi_{\overline{L}}} \operatorname{Tr}[\sigma_{\nu}^{2}]}{(2^{2m} - 1)^{2} (2^{2m} - 1)^{\xi_{\overline{L}}}} c_{1}^{2} R \sum_{\tau} t_{\tau} , \qquad (161)$$

where $R = \prod_{k=1}^{\xi} r_k^2$. Let us finally show that $\sum_{\tau} t_{\tau} \leq 2 \,\forall l, L$. We recall from Eq. (152) that the coefficients t_{τ} are obtained by integrating each block in $V(\theta)$ over the unitary group with the respect to the Haar measure. Each time a block is integrated one obtains four new tensors weighted by the coefficients η_i , with $i=1,\ldots,4$ such that $\sum_{\mu=1}^4 |\eta_\mu| \leqslant 1$ for all m. Consider now the average $\left\langle \text{Tr}[\Omega^i_{\boldsymbol{qp}}\Omega^j_{\boldsymbol{q'p'}}] \right\rangle_{V_p}$, once all the blocks have been integrated we find

$$\left\langle \text{Tr}[\Omega_{qp}^{i} \Omega_{q'p'}^{j}] \right\rangle_{V_R} = \sum_{\mu_1=1}^4 \eta_{\mu_1} \left(\sum_{\mu_2=1}^4 \eta_{\mu_2} \left(\dots \left(\sum_{\mu_m=1}^4 \eta_{\mu_m} \right) \right) \right) T_{\mu_1, \mu_2, \dots, \mu_m}(O),$$
 (162)

where μ_m is the number of averaged blocks, and where $T_{\mu_1,\mu_2,...,\mu_m}(O)$ is a tensor contraction of O. A similar equation can be obtained for $\left\langle \text{Tr}[\Omega^i_{qp}] \text{Tr}[\Omega^j_{q'p'}] \right\rangle_{V_-}$

$$\left\langle \text{Tr}[\Omega_{qp}^{i}] \text{Tr}[\Omega_{q'p'}^{j}] \right\rangle_{V_{R}} = \sum_{\mu'_{1}=1}^{4} \eta_{\mu'_{1}} \left(\sum_{\mu'_{2}=1}^{4} \eta_{\mu'_{2}} \left(\dots \left(\sum_{\mu'_{m}=1}^{4} \eta_{\mu'_{m}} \right) \right) \right) T_{\mu'_{1},\mu'_{2},\dots,\mu'_{m}}(O),$$
(163)

so that

$$\sum_{\tau} t_{\tau} = \sum_{\mu_1 = 1}^{4} \eta_{\mu_1} \left(\sum_{\mu_2 = 1}^{4} \eta_{\mu_2} \left(\dots \left(\sum_{\mu_m = 1}^{4} \eta_{\mu_m} \right) \right) \right) - \frac{1}{2^m} \sum_{\mu'_1 = 1}^{4} \eta_{\mu'_1} \left(\sum_{\mu'_2 = 1}^{4} \eta_{\mu'_2} \left(\dots \left(\sum_{\mu'_m = 1}^{4} \eta_{\mu'_m} \right) \right) \right). \tag{164}$$

Taking the absolute value on both side and using the fact that $\sum_{\mu=1}^{4} |\eta_{\mu}| \leq 1$, one gets $\sum_{\tau} t_{\tau} = |\sum_{\tau} t_{\tau}| \leq 1 + \frac{1}{2^{m}} \leq 2$. Therefore, by using $\operatorname{Tr}\left[\sigma_{\nu}^{2}\right]=2^{m}$, we have

$$\operatorname{Var}[\partial_{\nu}C] \leqslant \frac{2^{2m+\frac{n}{m}+l-L}}{(2^{2m}-1)^2(2^{2m}-1)^{\frac{n}{m}+l-L-1}}c_1^2R.$$

Moreover, we also find that

$$\frac{2^{2m+\frac{n}{m}+l-L}}{(2^{2m}-1)^2(2^{2m}-1)^{\frac{n}{m}+l-L-1}}c_1^2R = \frac{2^{2m}}{2^{2m}-1}\cdot\left(2^{2m-1}-\frac{1}{2}\right)^{L-l}\cdot\frac{2^{\frac{n}{m}}}{2^{2n}(1-2^{-2m})^{\frac{n}{m}}}c_1^2R,\tag{165}$$

and since $2^{2m-1} - \frac{1}{2} < 2^{2m-1}$ and $1 \leqslant \frac{1}{1-2^{-2m}} \leqslant \frac{4}{3}$, $\text{Var}[\partial_{\nu}C]$ can be upper bounded as $\text{Var}[\partial_{\nu}C] < F_n(L,l)$, where

$$F_n(L,l) = \frac{2^{2m + (2m-1)(L-l)}}{(2^{2m} - 1) \cdot 3^{\frac{n}{m}} \cdot 2^{(2-\frac{3}{m})n}} c_1^2 R.$$
(166)

B. Arbitrary N and \widehat{O}_{ik} is a traceless operators such that $\text{Tr}[\widehat{O}_{ik}^2] \leqslant 2^m$

We now consider the case when \hat{O}_{ik} is traceless. Specifically, we assume

$$\operatorname{Tr}\left[\widehat{O}_{ik}\right] = 0, \quad \text{and} \quad \operatorname{Tr}\left[\widehat{O}_{ik}^2\right] \leqslant 2^m.$$
 (167)

Note that if \widehat{O}_{ik} is a tensor product of Pauli operators then $\operatorname{Tr}\left[\widehat{O}_{ik}^2\right]=2^m$.

Proof. Let us first analyze the case of N=1. Combining Lemma 3 with Eqs. (153), and (154), we find

$$\langle \Omega_k \rangle_{W_{kL}} \leqslant \frac{2^m}{2^{2m} - 1} \left(\delta_{(\boldsymbol{p'}, \boldsymbol{q})_{S_k}} \delta_{(\boldsymbol{p}, \boldsymbol{q'})_{S_k}} - \frac{1}{2^m} \delta_{(\boldsymbol{p}, \boldsymbol{q})_{S_k}} \delta_{(\boldsymbol{p'}, \boldsymbol{q'})_{S_k}} \right) \leqslant \frac{2^m}{2^{2m} - 1} \delta_{(\boldsymbol{p'}, \boldsymbol{q})_{S_k}} \delta_{(\boldsymbol{p}, \boldsymbol{q'})_{S_k}}, \tag{168}$$

which yields

$$\prod_{k \in k_{\overline{L}}} \langle \Omega_k \rangle_{W_{kL}} \leqslant \frac{2^{\xi_{\overline{L}}m}}{(2^{2m} - 1)^{\xi_{\overline{L}}}} \prod_{k \in k_{\overline{L}}} \delta_{(\mathbf{p'}, \mathbf{q})_{S_k}} \delta_{(\mathbf{p}, \mathbf{q'})_{S_k}}.$$

$$(169)$$

Therefore, from (157), and (169), we can obtain

$$\operatorname{Var}\left[\partial_{\nu}C\right] \leqslant \frac{2^{2m-1}}{(2^{2m}-1)^{2}(2^{2m}-1)^{\xi_{\overline{\mathcal{L}}}}}c_{1}^{2} \cdot \frac{2^{\xi_{\overline{\mathcal{L}}}m}}{(2^{2m}-1)^{\xi_{\overline{\mathcal{L}}}}} \tag{170}$$

$$\times \sum_{\substack{\mathbf{p}\mathbf{q} \\ \mathbf{p}'\mathbf{q}'}} \sum_{\tau} t_{\tau} \Delta O_{\tau} \left(\prod_{k \in k_{\overline{L}}} \delta_{(\mathbf{p}',\mathbf{q})_{S_{k}}} \delta_{(\mathbf{p},\mathbf{q}')_{S_{k}}} \right) \delta_{(\mathbf{p},\mathbf{q})_{S_{\overline{\tau}}}} \delta_{(\mathbf{p}',\mathbf{q}')_{S_{\overline{\tau}}}} \delta_{(\mathbf{p},\mathbf{q}')_{S_{\tau}}} \delta_{(\mathbf{p}',\mathbf{q})_{S_{\tau}}} \left\langle \Delta \Psi_{\mathbf{p}\mathbf{q}}^{\mathbf{p}'\mathbf{q}'} \right\rangle_{V_{L}} . \tag{171}$$

Let us now consider the terms ΔO_{τ} from (125). It is straightforward to see that $\Delta O_{\tau} = 0$ if $S_{\tau_z} \neq \emptyset$, due to the fact that $\text{Tr}[\widehat{O}_{ik}] = 0$. Hence, let us define τ_p as the set of indexes such that $S_{\tau_z} = \emptyset$. Then, we have

$$\Delta O_{\tau} \leqslant \begin{cases} 2^{m(L-l+1)} & (\tau \in \tau_p) \\ 0 & (\tau \notin \tau_p) \end{cases} . \tag{172}$$

The latter implies

$$\sum_{\tau} t_{\tau} \Delta O_{\tau} \leqslant \sum_{\tau \in \tau_{p}} t_{\tau} \Delta O_{\tau} \leqslant 2 \times 2^{m(L-l+1)}, \qquad (173)$$

where we used the fact that $\sum t_{\tau} \leq 2$ (see Eq. (164) in the previous section),

According to Eqs. (132)–(135), the product $\left(\prod_{k \in k_{\overline{L}}} \delta_{(\boldsymbol{p'},\boldsymbol{q})_{S_k}} \delta_{(\boldsymbol{p},\boldsymbol{q'})_{S_k}}\right) \delta_{(\boldsymbol{p},\boldsymbol{q})_{S_{\overline{\tau}}}} \delta_{(\boldsymbol{p'},\boldsymbol{q'})_{S_{\overline{\tau}}}} \delta_{(\boldsymbol{p},\boldsymbol{q'})_{S_{\tau}}}$, leads to a Hilbert-Schmidt distances between two quantum states, which is always upper bounded by 2. We then find

$$\operatorname{Var}\left[\partial_{\nu}C\right] \leqslant \frac{2^{2m+1}}{(2^{2m}-1)^{2}(2^{2m}-1)^{\xi_{\overline{L}}}}c_{1}^{2} \cdot \frac{2^{\xi_{\overline{L}}m}}{(2^{2m}-1)^{\xi_{\overline{L}}}} \cdot 2^{m(L-l+1)}. \tag{174}$$

Since $n = m(L - l + 1) + m\xi_{\mathcal{L}}$, we can rewrite (174) as

$$\operatorname{Var}\left[\partial_{\nu}C\right] \leqslant \frac{2^{2m+n+1}(2^{2m}-1)^{2(L-l)}}{2^{4n}(1-2^{-2m})^{\frac{2n}{m}}}c_{1}^{2}.$$
(175)

Finally, noting that $2^{2m} - 1 \leqslant 2^{2m}$ and $1 \leqslant \frac{1}{1 - 2^{-2m}} \leqslant \frac{4}{3}$, we have

$$\operatorname{Var}\left[\partial_{\nu}C\right] \leqslant \frac{2^{2m(L-l+1)+1}}{3^{\frac{2n}{m}}2^{\left(3-\frac{4}{m}\right)n}}c_{1}^{2}.$$
(176)

Let us now consider the arbitrary N case, where the operator O can be expressed as

$$O = c_0 \mathbb{1} + \sum_{i=1}^{N} c_i O_i , \qquad (177)$$

and where each O_i can be expressed as $O_i = \widehat{O}_{i1} \otimes \widehat{O}_{i2} \otimes \cdots \otimes \widehat{O}_{i\xi}$ with \widehat{O}_{ik} satisfying (167). Here it is convinient to define $C_i = \text{Tr}[O_i V(\boldsymbol{\theta}) \rho V^{\dagger}(\boldsymbol{\theta})]$, so that $C = c_0 + \sum_i c_i C_i$. When computing the variance we now have to consider the cross terms arising from C_i , and C_j with $i \neq j$:

$$\operatorname{Var}[\partial_{\nu}C] = \langle (\partial_{\nu}C)^{2} \rangle_{V} = \sum_{i} c_{i}^{2} \langle (\partial_{\nu}C_{i})^{2} \rangle_{V} + \sum_{i \neq j} c_{i}c_{j} \langle \partial_{\nu}C_{i}\partial_{\nu}C_{j} \rangle_{V}.$$

$$(178)$$

First, let us remark that

$$\operatorname{Tr}\left[\widehat{O}_{ik}\right] = 0, \quad \text{and} \quad \operatorname{Tr}\left[\widehat{O}_{ik}\widehat{O}_{jk'}\right] \leqslant 2^{m}, \ \forall i, j, k, k' \quad \text{and} \quad \begin{cases} \Delta O_{\tau}^{ij} \leqslant 2^{m(L-l+1)} & (\tau \in \tau_{p}) \\ \Delta O_{\tau}^{ij} = 0 & (\tau \notin \tau_{p}) \end{cases}, \tag{179}$$

where ΔO_{τ}^{ij} was defined in (125), and where $\mathrm{Tr}\left[\widehat{O}_{ik}\widehat{O}_{jk'}\right]\leqslant 2^m$ follows from the fact that $\mathrm{Tr}\left[\widehat{O}_{ik}^2\right]\leqslant 2^m$ and $\operatorname{Tr}\left[\widehat{O}_{jk'}^2\right] \leqslant 2^m$. Hence, it is straigtforward to see that the upper bound in Eq. (176) also holds for the cross terms in (178), and we then have

$$Var[\partial_{\nu}C] \leqslant F_n(L,l). \tag{180}$$

where

$$F_n(L,l) = \frac{2^{2m(L-l+1)+1}}{3^{\frac{2n}{m}} 2^{(3-\frac{4}{m})n}} \sum_{ij} c_i c_j.$$
 (181)

Supplementary Note 8: Proofs of Corollaries

Proof of Corollary 1

Corollary 1. Consider the function $F_n(L, l)$.

(i) Let N=1 and let each \widehat{O}_{1k} be a non-trivial projector, as in case (i) of Theorem 1. If $c_1^2R\in\mathcal{O}(2^n)$ and if the number of layers $L \in \mathcal{O}(\text{poly}(\log(n)))$, then

$$F_n(L,l) \in \mathcal{O}\left(2^{-\left(1-\frac{1}{m}\log_2 3\right)n}\right),\tag{182}$$

which implies that $Var[\partial_{\nu}C]$ is exponentially vanishing in n if $m \ge 2$.

(ii) Let N be arbitrary, and let each \widehat{O}_{ik} satisfy $\text{Tr}[\widehat{O}_{ik}] = 0$ and $\text{Tr}[\widehat{O}_{ik}^2] \leqslant 2^m$, as in case (ii) of Theorem 1. If $N \in \mathcal{O}(2^n), c_i \in \mathcal{O}(1), and if the number of layers <math>L \in \mathcal{O}(\operatorname{poly}(\log(n))), then$

$$F_n(L,l) \in \mathcal{O}\left(\frac{1}{2^{\left(1-\frac{1}{m}\right)n}}\right),\tag{183}$$

which implies that $\operatorname{Var}[\partial_{\nu}C]$ is exponentially vanishing in n if $m \geq 2$.

Let us first consider case (i) in Theorem 1.

Proof. Let us assume $L \in \mathcal{O}(\text{poly}(\log(n)))$, so that we have $2^{(2m-1)(L-l)} \in \mathcal{O}(2^{\text{poly}(\log(n))})$. Here, note that

$$\lim_{n \to \infty} \left| \frac{\operatorname{poly}(\log(n))}{n} \right| = 0,$$

which means that n grows faster than the any polylogarithmic functions of n. $\mathcal{O}(\text{poly}(\log(n))) \subset \mathcal{O}(n)$. For a nonzero constant a, we can write $\mathcal{O}(|a|n) = \mathcal{O}(n)$, and we can choose

 $a = \frac{1}{m} \log_2(9/8)$. Therefore, we can also write $\mathcal{O}\left(2^{\text{poly}(\log(n))}\right) \subset \mathcal{O}\left((9/8)^{\frac{n}{m}}\right)$. In addition, if we have $c_1^2 R \in \mathcal{O}(2^n)$, from (166), one can obtain

$$F_n(L,l) \in \frac{1}{3^{\frac{n}{m}} 2^{\left(2-\frac{3}{m}\right)n}} \mathcal{O}\left((9/8)^{\frac{n}{m}}\right) \mathcal{O}\left(2^n\right) = \mathcal{O}\left(\frac{1}{2^{\left(1-\frac{1}{m}\log_2 3\right)n}}\right),\tag{184}$$

where $1 - \frac{1}{m} \log_2 3 > 0$ for $m \ge 2$. Hence the upper bound of $Var[\partial_{\nu} C_G]$ exponentially vanishing when $m \ge 2$.

Let us now consider case (ii) in Theorem 1.

Proof. We now have $2^{2m(L-l+1)+1} \in \mathcal{O}\left(2^{\text{poly}(\log(n))}\right) \subset \mathcal{O}\left((9/8)^{\frac{n}{m}}\right)$. We have from Eq. (181) that if $c_i, c_j \in \mathcal{O}(1)$, the following bound holds

$$F_n(L,l) \in \frac{1}{3^{\frac{2n}{m}} 2^{\left(3-\frac{4}{m}\right)n}} \mathcal{O}\left((9/8)^{\frac{n}{m}}\right) \mathcal{O}\left(2^{2n}\right) = \mathcal{O}\left(\frac{1}{2^{\left(1-\frac{1}{m}\right)n}}\right).$$

Hence, the upper bound of $Var[\partial_{\nu}C_G]$ exponentially vanishing when $m \geq 2$.

B. Proof of Corollary 2

Corollary 2. Consider the function $F_n(L,l)$. Let O be an operator of the form (116), as in Theorem 2. If at least one term $c_i^2 \epsilon(\rho_{k,k'}) \epsilon(\widehat{O}_i)$ in the sum in (118) vanishes no faster than $\Omega(1/\operatorname{poly}(n))$, and if the number of layers L is $\mathcal{O}(\log(n))$, then

$$G_n(L,l) \in \Omega\left(\frac{1}{\text{poly}(n)}\right)$$
 (185)

On the other hand, if at least one term $c_i^2 \epsilon(\rho_{k,k'}) \epsilon(\widehat{O}_i)$ in the sum in (118) vanishes no faster than $\Omega\left(1/2^{\text{poly}(\log(n))}\right)$, and if the number of layers is $\mathcal{O}(\text{poly}(\log(n)))$, then

$$G_n(L,l) \in \Omega\left(\frac{1}{2^{\text{poly}(\log(n))}}\right)$$
 (186)

Proof. Let us assume that at least one term $c_i^2 \epsilon(\rho_{k,k'}) \epsilon(\widehat{O}_i)$ in (118) vanishes no faster than $\Omega(1/\operatorname{poly}(n))$. Then, if we also assume $L \in \mathcal{O}(\log(n))$, we have $(2^m+1)^{-(L+l)} \in \Omega(1/\operatorname{poly}(n))$. The latter implies

$$G_n(L, l) \in \Omega\left(\frac{1}{\text{poly}(n)}\right) \Omega\left(\frac{1}{\text{poly}(n)}\right) = \Omega\left(\frac{1}{\text{poly}(n)}\right).$$

On the other hand, if at least one term $c_i^2 \epsilon(\rho_{k,k'}) \epsilon(\widehat{O}_i)$ in (118) vanishes no faster than $\Omega\left(1/2^{\text{poly}(\log(n))}\right)$, and if $L \in \mathcal{O}\left(\text{poly}(\log(n))\right)$, we have $(2^m+1)^{-(L+l)} \in \Omega\left(1/2^{\text{poly}(\log(n))}\right)$. Therefore, we obtain

$$G_n(L,l) \in \Omega\left(\frac{1}{2^{\text{poly}(\log(n))}}\right) \Omega\left(\frac{1}{2^{\text{poly}(\log(n))}}\right) = \Omega\left(\frac{1}{2^{\text{poly}(\log(n))}}\right).$$

Supplementary Note 9: Faithfulness of local cost function for Quantum autoencoder

Recall that the global cost function (C'_G) and local cost function (C'_L) for the quantum autoencoder are defined as

$$\begin{split} C_G' &= 1 - \mathrm{Tr} \left[|\mathbf{0}\rangle\!\langle \mathbf{0}| \rho_B^{\mathrm{out}} \right] \\ C_L' &= 1 - \frac{1}{n_B} \sum_{i=1}^{n_B} \mathrm{Tr} \left[\left(|0\rangle\!\langle \mathbf{0}|_j \otimes \mathbb{1}_{\overline{j}} \right) \rho_B^{\mathrm{out}} \right] \,. \end{split}$$

We relate the C'_L and C'_G cost functions in the following proposition. Because this proposition establishes that C'_L and C'_G vanish under the same conditions, and because C'_G is faithful [9], this in turn proves that C'_L is a faithful cost function.

Proposition 3. The cost functions for the quantum autoencoder satisfy

$$C_L' \leqslant C_G' \leqslant n_B C_L'. \tag{187}$$

Proof. Let us first prove $C'_L \leqslant C'_G$. Given the state ρ_B^{out} , we can define E_j as the event of qubit j being measured on the $|0\rangle_j$ state, such that the probability of E_j is given by $\Pr(E_j) = \text{Tr}\left[\widehat{O}_j^L \rho_B^{\text{out}}\right]$, where $\widehat{O}_j^L = |0\rangle\langle 0|_j \otimes \mathbb{1}_{\overline{j}}$. Then, we can write

$$C_G' = 1 - \Pr\left(\bigcap_{j=1}^{n_B} E_j\right) \tag{188}$$

Similarly, for the local cost function, we have

$$C'_{L} = 1 - \frac{1}{n_B} \sum_{i=1}^{n_B} \Pr(E_i).$$
 (189)

Then, it is known that for any set of events $\{E_1, \dots, E_{n_B}\}$, the following property always holds

$$1 - \Pr\left(\bigcap_{j=1}^{n_B} E_j\right) \ge \frac{1}{n_B} \sum_{j=1}^{n_B} \left(1 - \Pr\left(E_j\right)\right). \tag{190}$$

From the definition of C'_G and C'_L in Eqs. (188)– (189), and from Eq. (190) we have

$$C_L' \leqslant C_G'. \tag{191}$$

Next, let us prove $C'_G \leq n_B C'_L$. Since for any set of events $\{E_1, \dots, E_{n_B}\}$, we have

$$1 - \Pr\left(\bigcap_{j=1}^{n_B} E_j\right) \leqslant \sum_{j=1}^{n_B} \left(1 - \Pr\left(E_j\right)\right). \tag{192}$$

By definition, we finally have

$$C_G' \leqslant n_B C_L'. \tag{193}$$

Combining Eqs. (191) and (193), we get (187), which indicates $C'_L = 0 \iff C'_G = 0$.