Quantum machine learning: on the design, trainability and noise-robustness of near-term algorithms

Skolik, A.

Citation

Skolik, A. (2023, December 7). *Quantum machine learning: on the design, trainability and noise-robustness of near-term algorithms*. Retrieved from https://hdl.handle.net/1887/3666138

Appendix

Layerwise learning for quantum neural networks

As alluded to in Section 4.1, LL and CDL perform similarly in a perfect simulation scenario, where we assume neither shot nor hardware noise. Figure 1 a) shows a comparison of LL and CDL under perfect conditions, i.e. infinite number of measurements and a batch size that corresponds to the number of samples, which enables computation of exact gradients. Here, the magnitude of gradients doesn't affect the learning process severely, as the Adam optimizer uses adaptive learning rates for each parameter and can therefore handle different ranges of gradient magnitudes well as long as there is some variance in the computed gradients. In this regime, both approaches show similar performance.

The convergence rate of a PQC increases proportionally to the number of parameters in a model [188], so the number of experiment repetitions is almost equal for LL and CDL. LL has less parameters and needs more epochs to converge due to this, whereas CDL needs more calls to the quantum device for one update step, but in turn needs less epochs to converge. In terms of cross entropy, both LL and CDL converge to a value of roughly 0.51. The corresponding test error of all approaches, except for the randomly initialized CDL, reaches almost 0 but doesn't converge there and settles around an error of roughly 0.1 eventually, as seen in Figure 1 b).
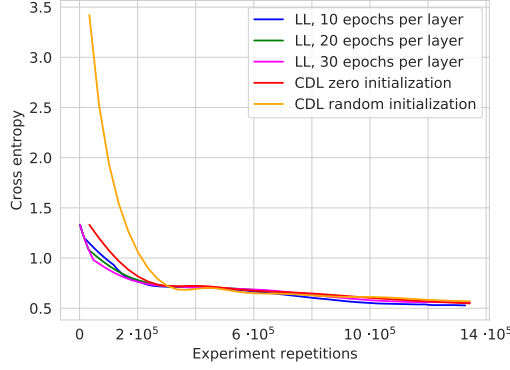
(a) cross entropy
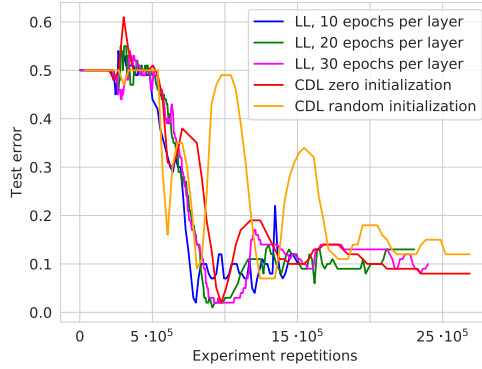
(b) test error

Figure 1: a) Cross entropy of LL and CDL during training with exact gradient calculation corresponding to infinite number of measurements. When one assumes the unphysical situation of infinite measurements ($m = \infty$) all methods seem to perform similarly. In particular, we compare LL to CDL with zero and random initialization, where the initial parameters for the latter are chosen uniformly from $[0, 2\pi)$. The hyperparameters for all configurations were set to $m = \infty$, $b = 100$ and $\eta = 0.01$. (For computing the number of experiment repetitions as defined in Section 4.2.3, we drop m.) b) Test error corresponding to the runs shown in Figure 1. This further supports the observation that when one allows unphysical, arbitrary precision queries($m = \infty$), all tuned training strategies seem to perform similarly.

Quantum agents in the Gym: A variational quantum algorithm for deep Q-learning
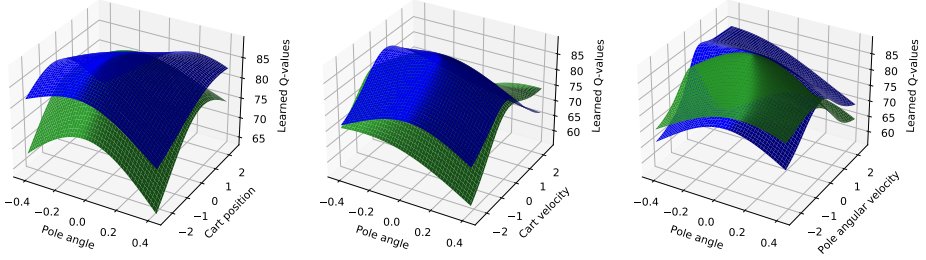
Visualization of a learned Q-function

Figure 2: Visualization of the approximate Q-function learned by a quantum Q-learning agent solving Cart Pole. Due to the 4 dimensions of the state space in Cart Pole, we represent the Q-values associated to the actions "left" (green) and "right" (blue) on 3 subspaces of the state space by fixing unrepresented dimensions to 0 in each plot. As opposed to the analogue values (i.e., unnormalized policy) learned by policy-gradient PQC agents in this environment [150], the approximate Q-values appear nicely-behaved, likely due to the stronger constraints that Q-learning has on well-performing function approximations.

Model hyperparameters

In the following, we give a detailed list of the hyperparameters for each configuration in fig. 5.3, fig. 5.4, fig. 5.5, fig. 5.6 and fig. 5.7. The hyperparameters that we searched over for each model were the following (see explanations of each hyperparameter in table 1):

- *Frozen Lake v0*: update model, update target model, η

- *Cart Pole v0, quantum model*: batch size, update model, update target model, η, train w_d, train w_o, η_{w_d}, η_{w_o}

- *Cart Pole v0, classical model*: number of units per layer, batch size, update model, update target model, η

	Hyperparameter explanation
qubits	number of qubits in circuit
layers	number of layers
γ	discount factor for Q-learning
train w_d	train weights on the model input as defined in section 5.1.1
train w_o	train weights on the model output as defined in section 5.1.2
η	model parameter learning rate
ηw_d	input weight learning rate
ηw_o	output weight learning rate
batch size	number of samples shown to optimizer at each update
ϵ_{init}	initial value for ϵ-greedy policy
ϵ_{dec}	decay of ϵ for ϵ-greedy policy
ϵ_{min}	minimal value of ϵ for ϵ-greedy policy
update model	time steps after which model is updated
update target model	time steps after which model parameters are copied to target model
size of replay memory	size of memory for experience replay
data re-uploading	use data re-uploading as defined in section 5.1.1

Table 1: Description of hyperparameters considered in this work

	Frozen Lake v0, fig. 5.3	Cart Pole v0, optimal	Cart Pole v0, sub-optimal
qubits	4	4	4
layers	5, 10, 15	5	5
γ	0.8	0.99	0.99
train w_d	no	yes, no	yes, no
train w_o	no	yes, no	yes, no
η	0.001	0.001	0.001
ηw_d	–	0.001	0.001
ηw_o	–	0.1	0.1
batch size	11	16	16
ϵ_{init}	1	1	1
ϵ_{dec}	0.99	0.99	0.99
ϵ_{min}	0.01	0.01	0.01
update model	5	1	10
update target model	10	1	30
size of replay memory	10000	10000	10000
data re-uploading	no	yes, no	yes, no

Table 2: Hyperparameter settings of PQCs in fig. 5.3, fig. 5.4 and fig. 5.5

layers	5	10	15	20	25	30
qubits	4	4	4	4	4	4
γ	0.99	0.99	0.99	0.99	0.99	0.99
train w_d	yes	yes	yes	yes	yes	yes
train w_o	yes	yes	yes	yes	yes	yes
η	0.001	0.001	0.001	0.001	0.001	0.001
η_{w_d}	0.001	0.001	0.001	0.001	0.001	0.001
η_{w_o}	0.1	0.1	0.1	0.1	0.1	0.1
batch size	16	64	32	16	64	16
ϵ_{init}	1	1	1	1	1	1
ϵ_{dec}	0.99	0.99	0.99	0.99	0.99	0.99
ϵ_{min}	0.01	0.01	0.01	0.01	0.01	0.01
update model	1	10	10	10	10	10
update target model	1	30	30	30	30	30
size of replay memory	10000	10000	10000	10000	10000	10000
data re-uploading	yes	yes	yes	yes	yes	yes

Table 3: Hyperparameter settings of PQCs in fig. 5.6 a)

units in hidden layers	(10, 10)	(15, 15)	(20, 20)	(24, 24)	(30, 30)	(64, 64)
γ	0.99	0.99	0.99	0.99	0.99	0.99
η	0.001	0.001	0.001	0.001	0.001	0.001
batch size	64	16	64	64	64	16
ϵ_{init}	1	1	1	1	1	1
ϵ_{dec}	0.99	0.99	0.99	0.99	0.99	0.99
ϵ_{min}	0.01	0.01	0.01	0.01	0.01	0.01
update model	1	1	1	1	1	1
update target model	1	1	1	1	1	1
size of replay memory	10000	10000	10000	10000	10000	10000

Table 4: Hyperparameter settings of NNs in fig. 5.6 b)

# Equivariant quantum circuits for learning on weighted graphs

Additional results on statistical significance of comparison between EQC and NEQC

To make statements on the statistical significance of the difference between the performance of the EQC and NEQC shown in Figure 6.5, we perform a two-sample t-test on the two models for the same instance sizes (i.e., for the data in the two boxes for each instance size) with the null hypothesis that the averages of the two distributions are the same. Based on this, we compute p-values to quantify the statistical significance of the differences between models.
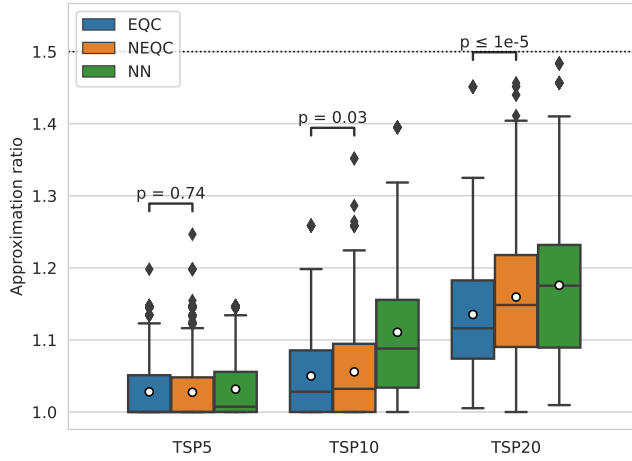
Figure 3 a) shows p-values for the depth-one EQCs and NEQCs from Figure 6.5 b). For the 5-city instances, we can not reject the null hypothesis. Indeed, it is already visible by looking at the boxes that the distributions are very similar, which can be expected as the number of permutations of a graph with five vertices is small. However, as we scale up the instance size to ten cities, the corresponding p-value is much smaller than 0.05, which means that we can reject the null hypothesis that the two distributions have the same average with high confidence. This is also the case for the instances with twenty cities, where the p-value is less than 0.01.

Figure 3 b) shows p-values for the depth four EQCs and NEQCs from Figure 6.5 d). Again, the p-value of the 5-city instances is very high with 0.74, so that we can not reject the null hypothesis. Also similarly to the above, the p-values get smaller as we scale up the instance size. For the depth-four ansatzes, the p-value is smallest for the twenty city instances, with a value much smaller than 0.05.

To provide additional insight, we also plot the means and their standard error for both the 1-layer (EQC-1, NEQC-1) and 4-layer (EQC-4, NEQC-4) models in Figure 6.5. As a rule of thumb, one can expect that when the error bars given by the standard errors of two means do not overlap, the p-value can be smaller than 0.05, while in the case that they do overlap, the p-value is likely much larger. The error bars in Figure 4 are in line with this statement, where we see that the error bars for the five-city instances overlap for both circuit depths, while this is not the case for the larger instance sizes and in addition the distance between the means increases for those instance sizes. Remarkably, we also see that the difference
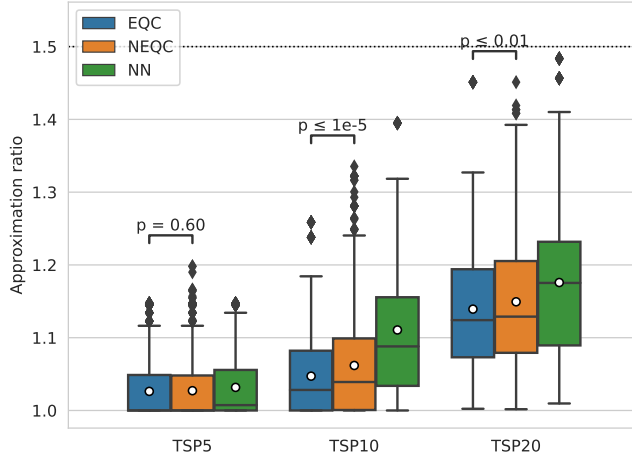
(a) one layer

(b) four layers

Figure 3: P-values for comparison of EQCs and NEQCs at depth one and four from Figure 6.5 b) and d).
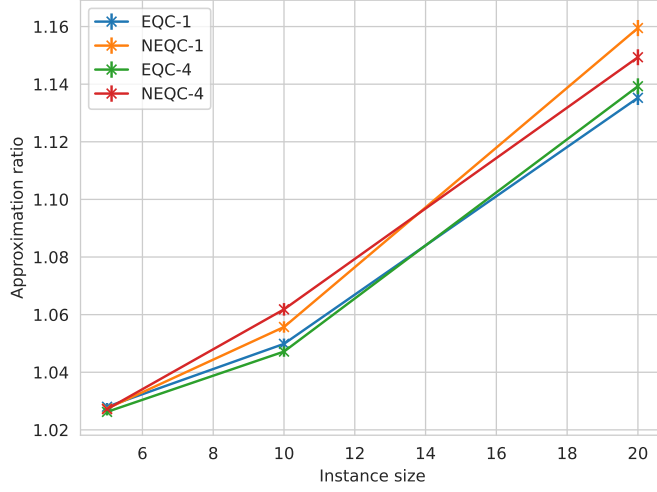
Figure 4: Mean and standard error of the mean for the one- and four-layer EQCs and NEQCs in Figure 6.5 b), d).

between the EQC at depths one and four is very small, and that increasing the circuit depth does not provide much benefit on this learning task.

Robustness of quantum reinforcement learning under hardware errors

Gaussian Noise Analysis

In this Appendix we perform the noise analysis of a scalar function whose parameters are corrupted by independently distributed Gaussian perturbations. Let $f : \mathbb{R}^M \to \mathbb{R}$ be the function under investigation, whose parameters $\boldsymbol{\theta} = (\theta_1, \ldots, \theta_M) \in \mathbb{R}^M$ are corrupted by a Gaussian noise $\theta_i \to \theta_i + \delta\theta_i$ with zero mean and variance σ^2, i.e.

$$
\begin{aligned}
&\delta\theta_i \sim \mathcal{N}(0, \sigma^2) \quad \forall i = 1, \ldots, M\,, \\
&\mathbb{E}[\delta\theta_i] = 0\,, \\
&\mathbb{E}[\delta\theta_i \delta\theta_j] = \sigma^2 \delta_{ij}\,.
\end{aligned}
\tag{1}
$$

Since the perturbations are independently distributed and Gaussian, all higher order moments can be evaluated starting from two-point correlators of the form $\mathbb{E}[\delta\theta_i \delta\theta_j]$, as dictated by *Wick's formulas* for multivariate normal distributions [305]

$$
\begin{aligned}
&\mathbb{E}[\delta\theta_{i_1} \cdots \delta\theta_{i_{2n+1}}] = 0\,, \\
&\mathbb{E}[\delta\theta_{i_1} \cdots \delta\theta_{i_{2n}}] = \sum_{\mathcal{P}} \mathbb{E}[\delta\theta_{k_1} \delta\theta_{k_2}] \cdots \mathbb{E}[\delta\theta_{k_{2n-1}} \delta\theta_{k_{2n}}]\,,
\end{aligned}
\tag{2}
$$

where with $\mathcal{P}$ we denote all the possible distinct $(2n-1)!!$ pairings of the n variables, as these can be used to express all higher order even moments in terms of products of second moments. Note that all the terms involving an odd number of perturbations $\delta\theta_i$ vanish, and only even moments remain. For example, expression (2) for the fourth-order moment ($n = 4$) amounts to

$$
\begin{aligned}
\mathbb{E}[\delta\theta_i \delta\theta_j \delta\theta_k \delta\theta_m] &= \mathbb{E}[\delta\theta_i \delta\theta_j]\,\mathbb{E}[\delta\theta_k \delta\theta_m] + \mathbb{E}[\delta\theta_i \delta\theta_k]\,\mathbb{E}[\delta\theta_j \delta\theta_m] + \mathbb{E}[\delta\theta_i \delta\theta_m]\,\mathbb{E}[\delta\theta_j \delta\theta_k] \\
&= \sigma^4\big(\delta_{ij}\delta_{km} + \delta_{ik}\delta_{jm} + \delta_{im}\delta_{jk}\big)\,.
\end{aligned}
\tag{3}
$$

We now proceed considering the multi dimensional Taylor expansion of the function

$f(\boldsymbol{\theta} + \delta\boldsymbol{\theta})$ around the noise-free point. Up to arbitrary order, this reads

$$f(\boldsymbol{\theta} + \delta\boldsymbol{\theta}) = f(\boldsymbol{\theta}) + \sum_{i=1}^{M} \frac{\partial f(\boldsymbol{\theta})}{\partial \theta_i} \delta\theta_i + \frac{1}{2!} \sum_{i,j=1}^{M} \frac{\partial^2 f(\boldsymbol{\theta})}{\partial \theta_i \partial \theta_j} \delta\theta_i \delta\theta_j$$

$$+ \frac{1}{3!} \sum_{i,j,k=1}^{M} \frac{\partial^3 f(\boldsymbol{\theta})}{\partial \theta_i \partial \theta_j \partial \theta_k} \delta\theta_i \delta\theta_j \delta\theta_k + \dots . \quad (4)$$

where we used the equal sign because we are considering the full Taylor series, and we assume that this converges to the true function (this statement can be made precise by showing that the remainder term of the expansion goes to zero as the order of expansion goes to infinity).

Before proceeding, we simplify the notation to make the calculation of the Taylor expansion easier to follow. First, we denote the partial derivatives with respect to parameter θ_i as $\partial_i := \partial/\partial \theta_i$, and similarly for higher order derivatives, for example $\partial_{ij} = \partial^2/\partial \theta_i \partial \theta_j$. Also, we suppress the explicit dependence of the function on $\boldsymbol{\theta}$, using the short-hand f instead of $f(\boldsymbol{\theta})$. At last, we make use of Einstein' summation notation where repeated indexes imply summation.

With this setup, using Eqs. (1), (2) and (3) in (4), one can evaluate the expectation value of the function over the perturbations' distributions as

$$\mathbb{E}[f(\boldsymbol{\theta} + \delta\boldsymbol{\theta})] = f(\boldsymbol{\theta}) + \partial_i f\, \mathbb{E}[\delta\theta_i] + \frac{1}{2}\partial_{ij} f\, \mathbb{E}[\delta\theta_i \delta\theta_j] + \frac{1}{3!}\partial_{ijk} f\, \mathbb{E}[\delta\theta_i \delta\theta_j \delta\theta_k]$$

$$+ \frac{1}{4!}\partial_{ijkm} f\, \mathbb{E}[\delta\theta_i \delta\theta_j \delta\theta_k \delta\theta_m] + \dots$$

$$= f(\boldsymbol{\theta}) + \frac{\sigma^2}{2}\partial_{ij} f\, \delta_{ij} + \frac{\sigma^4}{4!}\partial_{ijkm} f\, (\delta_{ij}\delta_{km} + \delta_{ik}\delta_{jm} + \delta_{im}\delta_{jk}) + \dots$$

$$= f(\boldsymbol{\theta}) + \frac{\sigma^2}{2}\sum_i \frac{\partial^2 f}{\partial \theta_i^2} + \frac{\sigma^4}{4!}3\sum_{ij} \frac{\partial^4 f}{\partial \theta_i^2 \partial \theta_j^2} + \dots$$

$$(5)$$

where in the last line we simplified the fourth order term as

$$\mathbb{E}[f^{(4)}] = \frac{\sigma^4}{4!}\partial_{ijkm} f\left(\delta_{ij}\delta_{km} + \delta_{ik}\delta_{jm} + \delta_{im}\delta_{jk}\right)$$

$$= \frac{\sigma^4}{4!}\left(\sum_{ik} \frac{\partial^4 f}{\partial \theta_i^2 \partial \theta_k^2} + \sum_{ij} \frac{\partial^4 f}{\partial \theta_i^2 \partial \theta_j^2} + \sum_{im} \frac{\partial^4 f}{\partial \theta_i^2 \partial \theta_m^2}\right)$$

$$= \frac{\sigma^4}{4!}3\sum_{ij} \frac{\partial^4 f}{\partial \theta_i^2 \partial \theta_j^2}.$$

Since the expectation values involving an odd number of perturbations vanish, only the even order terms survive, and these can be expressed as

$$\mathbb{E}[f^{(2n)}] = \frac{\sigma^{2n}}{(2n)!}(2n-1)!! \sum_{i_1,\ldots,i_n} \frac{\partial^{2n} f(\boldsymbol{\theta})}{\partial \theta_{i_1}^2 \ldots \partial \theta_{i_n}^2} . \tag{6}$$

where the coefficient $(2n-1)!!$ is the number of distinct pairings of $2n$ objects, which comes from Eq. Equation (1).

Thus, the full Taylor series can be formally written as

$$\mathbb{E}[f(\boldsymbol{\theta} + \delta\boldsymbol{\theta})] = f(\boldsymbol{\theta}) + \sum_{n=1}^{\infty} \frac{\sigma^{2n}}{(2n)!}(2n-1)!! \sum_{i_1,\ldots,i_n=1}^{M} \frac{\partial^{2n} f(\boldsymbol{\theta})}{\partial \theta_{i_1}^2 \ldots \partial \theta_{i_n}^2} \tag{7}$$

$$= f(\boldsymbol{\theta}) + \frac{\sigma^2}{2} \operatorname{Tr}[H(\boldsymbol{\theta})] + \sum_{n=2}^{\infty} \frac{\sigma^{2n}}{(2n)!}(2n-1)!! \sum_{i_1,\ldots,i_n=1}^{M} \frac{\partial^{2n} f(\boldsymbol{\theta})}{\partial \theta_{i_1}^2 \ldots \partial \theta_{i_n}^2} \tag{8}$$

where we introduced the Hessian matrix $H(\boldsymbol{\theta})$, whose elements are given by $[H(\boldsymbol{\theta})]_{ij} = \partial_{ij} f(\boldsymbol{\theta})$, and we see that this term represent the first non-vanishing correction to the function caused by the perturbation.

Our goal is to bound the absolute error

$$\varepsilon_{\boldsymbol{\theta}} := |\mathbb{E}[f(\boldsymbol{\theta} + \delta\boldsymbol{\theta})] - f(\boldsymbol{\theta})| = \left| \sum_{n=1}^{\infty} \frac{\sigma^{2n}}{(2n)!}(2n-1)!! \sum_{i_1,\ldots,i_n=1}^{M} \frac{\partial^{2n} f(\boldsymbol{\theta})}{\partial \theta_{i_1}^2 \ldots \partial \theta_{i_n}^2} \right| \tag{9}$$

caused by the gaussian noise, and we can do that by using the property that all the derivatives of most PQC (Parametrized Quantum Circuit) are bounded. In fact, for those circuits for which a *parameter-shift* rule holds [? ?], one can show that any derivative of the function $f(\boldsymbol{\theta}) = \langle O \rangle = \operatorname{Tr}\left[O\, U(\boldsymbol{\theta}) |0\rangle\langle 0|\, U^{\dagger}(\boldsymbol{\theta}) \right]$ obeys

$$\left| \frac{\partial^{\alpha_1 + \ldots \alpha_M} f(\boldsymbol{\theta})}{\partial \theta_1^{\alpha_1} \ldots \partial \theta_M^{\alpha_M}} \right| \leq \|O\|_{\infty} , \tag{10}$$

where $\|O\|_{\infty}$ is the infinity norm of the observable, namely its largest absolute eigenvalue. We give a proof of this below in Sec. 8.

Plugging this in Eq. (9), we can obtain an upper bound to the error $\varepsilon_{\boldsymbol{\theta}}$ as desired. Indeed, remembering that for even numbers the double factorial can be expressed

as $(2n-1)!! = (2n)!/(2^n n!)$, it holds

$$
\begin{aligned}
\varepsilon_{\boldsymbol{\theta}} &= \left| \sum_{n=1}^{\infty} \frac{\sigma^{2n}}{(2n)!}(2n-1)!! \sum_{i_1,\ldots,i_n=1}^{M} \frac{\partial^{2n} f(\boldsymbol{\theta})}{\partial\theta_{i_1}^2 \ldots \partial\theta_{i_n}^2} \right| \qquad (11) \\
&\leq \sum_{n=1}^{\infty} \frac{\sigma^{2n}}{(2n)!}(2n-1)!! \sum_{i_1,\ldots,i_n=1}^{M} \underbrace{\left| \frac{\partial^{2n} f(\boldsymbol{\theta})}{\partial\theta_{i_1}^2 \ldots \partial\theta_{i_n}^2} \right|}_{\leq \|O\|_\infty} \\
&\leq \sum_{n=1}^{\infty} \frac{\sigma^{2n}}{(2n)!}(2n-1)!! \, \|O\|_\infty \, M^n \qquad (12) \\
&= \|O\|_\infty \sum_{n=1}^{\infty} \frac{1}{(2n)!}\frac{(2n)!}{2^n n!}(\sigma^2 M)^n = \|O\|_\infty \sum_{n=1}^{\infty} \frac{(M\sigma^2/2)^n}{n!} \\
&= \|O\|_\infty \left(e^{\sigma^2 M/2} - 1 \right) \\
&\implies \varepsilon_{\boldsymbol{\theta}} = |\mathbb{E}[f(\boldsymbol{\theta}+\delta\boldsymbol{\theta})] - f(\boldsymbol{\theta})| \leq \|O\|_\infty \left(e^{M\sigma^2/2} - 1 \right), \qquad (13)
\end{aligned}
$$

where in the last line we used the definition of the exponential function $e^x = \sum_{n=0}^{\infty} \frac{x^n}{n!}$.

One can see that the noise variance σ^2 must scale as the inverse of the number of parameters $\sigma^2 \in \mathcal{O}(M^{-1})$ in order to have small deviations induced by the noise. Also, note that since the difference between the noise-free function $f(\boldsymbol{\theta})$ and its perturbed version $f(\boldsymbol{\theta}+\delta\boldsymbol{\theta})$ cannot be larger than twice the maximum eigenvalue of O, $|f(\boldsymbol{\theta}+\delta\boldsymbol{\theta}) - f(\boldsymbol{\theta})| \leq |f(\boldsymbol{\theta}+\delta\boldsymbol{\theta})| + |f(\boldsymbol{\theta})| = 2\|O\|_\infty$, the bound (11) is informative only as long as $\exp[M\sigma^2/2] - 1 < 2$.

It is worth noticing that an identical procedure can be used to bound the average error obtained by approximating the perturbed function with its first non-vanishing correction given by the Hessian. Indeed, starting from Eq. (8) are repeating the same calculation from above, one obtains

$$
\left| \mathbb{E}[f(\boldsymbol{\theta}+\delta\boldsymbol{\theta})] - f(\boldsymbol{\theta}) - \frac{\sigma^2}{2}\mathrm{Tr}[H(\boldsymbol{\theta})] \right| \leq \|O\|_\infty \left(e^{M\sigma^2/2} - 1 - \frac{M\sigma^2}{2} \right). \qquad (14)
$$

Parameter-Shift rule and bounds to the derivatives

Let $f(\boldsymbol{\theta}) = \mathrm{Tr}\left[O\, U(\boldsymbol{\theta}) |0\rangle\langle 0| \, U^\dagger(\boldsymbol{\theta}) \right]$ be the expectation value of an observable O on the parametrized state $|\psi(\boldsymbol{\theta})\rangle = U(\boldsymbol{\theta})|0\rangle$ obtained with a parametrized quantum circuit $U(\boldsymbol{\theta})$. When the variational parameters $\boldsymbol{\theta} \in \mathbb{R}^M$ enter in the quantum circuit via rotation gates of the form $V(\theta_i) = \exp[-i\theta_i P/2]$ with $P^2 = \mathbb{1}$ being

Pauli operators, then the *parameter-shift* rule can be used to evaluate gradients of the expectation value [39, 33], as described in Section 2.2.1.1,

$$\frac{\partial f(\boldsymbol{\theta})}{\partial \theta_i} = \frac{1}{2}\left(f\left(\boldsymbol{\theta} + \frac{\pi}{2}\boldsymbol{e_i}\right) - f\left(\boldsymbol{\theta} - \frac{\pi}{2}\boldsymbol{e_i}\right)\right), \tag{15}$$

where $\boldsymbol{e_i}$ is the unit vector with zero entries and a one in the $i-$th position corresponding to angle θ_i. Similarly, by applying the parameter-shift rule twice one can express second order derivatives as follows using four evaluations of the circuit [280, 306]

$$\frac{\partial^2 f(\boldsymbol{\theta})}{\partial \theta_i \theta_j} = \frac{1}{2}\left[\frac{\partial}{\partial \theta_i} f\left(\boldsymbol{\theta} + \frac{\pi}{2}e_j\right) - \frac{\partial}{\partial \theta_i} f\left(\boldsymbol{\theta} - \frac{\pi}{2}e_j\right)\right] \tag{16}$$

$$= \frac{1}{4}[f(\boldsymbol{\theta} + \frac{\pi}{2}\boldsymbol{e_j} + \frac{\pi}{2}\boldsymbol{e_i}) - f(\boldsymbol{\theta} + \frac{\pi}{2}\boldsymbol{e_j} - \frac{\pi}{2}\boldsymbol{e_i}) \tag{17}$$

$$-f\left(\boldsymbol{\theta} - \frac{\pi}{2}\boldsymbol{e_j} + \frac{\pi}{2}\boldsymbol{e_i}\right) + f\left(\boldsymbol{\theta} - \frac{\pi}{2}\boldsymbol{e_j} - \frac{\pi}{2}\boldsymbol{e_i}\right)]. \tag{18}$$

In particular, for the diagonal elements $i = j$, one has

$$\begin{aligned}\frac{\partial^2 f(\boldsymbol{\theta})}{\partial \theta_i^2} &= \frac{1}{4}[f(\boldsymbol{\theta} + \pi\boldsymbol{e_i}) - 2f(\boldsymbol{\theta}) + f(\boldsymbol{\theta} - \pi\boldsymbol{e_i})] \\ &= \frac{1}{2}[f(\boldsymbol{\theta} + \pi\boldsymbol{e_i}) - f(\boldsymbol{\theta})], \end{aligned} \tag{19}$$

where we used the fact that $f(\boldsymbol{\theta} + \pi\boldsymbol{e_i}) = f(\boldsymbol{\theta} - \pi\boldsymbol{e_i})$. This last equality can be seen intuitively from the 2π periodicity of the rotation gates or by direct evaluation. In fact, let $U(\boldsymbol{\theta}) = U_2 \exp[-i\theta_i P_i/2] U_1$ be a factorization of the parametrized unitary where we isolated the dependence on the parameter θ_i to be shifted. Then, since $\exp[-i\,2\pi P/2] = \cos \pi\,\mathbb{I} - i \sin \pi P = -\mathbb{I}$, one has

$$\begin{aligned}|\psi(\boldsymbol{\theta} - \pi\boldsymbol{e_i})\rangle &= U_2 \exp[-i(\theta_i - \pi)P_i/2]\, U_1\,|0\rangle \\ &= U_2 \exp[-i(\theta_i - \pi)P_i/2]\underbrace{-\exp[-i\,2\pi\,P_i/2]}_{\mathbb{I}}U_1\,|0\rangle \\ &= -U_2 \exp[-i(\theta_i - \pi + 2\pi)P_i/2]U_1\,|0\rangle \\ &= -\,|\psi(\boldsymbol{\theta} + \pi\boldsymbol{e_i})\rangle\,, \end{aligned} \tag{20}$$

and thus $\langle\psi(\boldsymbol{\theta} - \pi\boldsymbol{e_i})|O|\psi(\boldsymbol{\theta} - \pi\boldsymbol{e_i})\rangle = \langle\psi(\boldsymbol{\theta} + \pi\boldsymbol{e_i})|O|\psi(\boldsymbol{\theta} + \pi\boldsymbol{e_i})\rangle$.

Hence, using Eq. (19) it is possible to estimate the diagonal elements of the Hessian matrix with just two different evaluations of the quantum circuit.

By repeated application of the parameter-shift rule one can also evaluate arbitrary higher-order derivatives as linear combinations of circuit evaluations [280, 51]. Let $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_M) \in \mathbb{N}^M$ be a multi-index keeping track of the orders of derivatives, and let $|\boldsymbol{\alpha}| = \sum_{i=1}^{M} \alpha_i$. Then

$$\partial^{\boldsymbol{\alpha}} f(\boldsymbol{\theta}) := \frac{\partial^{|\boldsymbol{\alpha}|} f(\boldsymbol{\theta})}{\partial \theta_1^{\alpha_1} \ldots \partial \theta_M^{\alpha_M}} = \frac{1}{2^{|\boldsymbol{\alpha}|}} \sum_{m=1}^{2^{|\boldsymbol{\alpha}|}} s_m f(\tilde{\boldsymbol{\theta}}_m), \tag{21}$$

where $s_m \in \{\pm 1\}$ are signs, and $\tilde{\boldsymbol{\theta}}_m$ are angles obtained by accumulation of shifts along multiple directions.

Since the output of any circuit evaluation is bounded by the infinity norm (i.e, the largest absolute eigenvalue) of the observable $\|O\|_\infty = \max\{|o_i|, O = \sum_i o_i |o_i\rangle\langle o_i|\}$

$$|f(\boldsymbol{\theta})| = |\text{Tr}[O \rho(\boldsymbol{\theta})]| \le \|O\|_\infty \|\rho(\boldsymbol{\theta})\|_1 = \|O\|_\infty \quad \forall \boldsymbol{\theta} \in \mathbb{R}^M, \tag{22}$$

then one can bound the sum in Eq. (21) simply as

$$|\partial^{\boldsymbol{\alpha}} f(\boldsymbol{\theta})| \le \frac{1}{2^{|\boldsymbol{\alpha}|}} \sum_{m=1}^{2^{|\boldsymbol{\alpha}|}} \left| f(\tilde{\boldsymbol{\theta}}_m) \right| \le \|O\|_\infty. \tag{23}$$

Average value of the Hessian of random PQCs

In this section we derive the formulas (7.16) and (7.17) for the expected value of the Hessian as shown in the main text. Consider a system of n qubits and a parametrized quantum circuit with unitary $U(\boldsymbol{\theta}) \in \mathcal{U}(2^n)$, where $\mathcal{U}(2^n)$ is the group of unitary matrices of dimension 2^n. Given a set of parameter vectors $\{\boldsymbol{\theta}_1, \boldsymbol{\theta}_2, \ldots, \boldsymbol{\theta}_K\}$, one can construct the corresponding set of unitaries $\mathbb{U} = \{U_1, U_2, \ldots, U_K\}$, with $U_i = U(\boldsymbol{\theta}_i)$ and clearly $\mathbb{U} \in \mathcal{U}(2^n)$.

It is now well known that sampling a parametrized quantum circuit from a random assignment of the parameters is approximately equal to drawing a random unitary from the Haar distribution, a phenomenon which is at the root of the insurgence of barren plateaus (BPs) [48, 229, 44]. Specifically, it is numerically observed that parametrized quantum circuits behave like unitary 2-designs, that is averaging over unitaries U_i sampled from $\mathbb{U}$ yields the same result of averaging over Haar-random unitaries, up until second order moments.

As standard in the literature regarding BPs, in the following we assume that the considered parametrized unitaries (and parts of them) are indeed 2-designs, and so

we make use of the following relations for integration over random unitaries [289, 307, 288, 48, 44]

$$\mathbb{E}_U[UAU^\dagger] = \int d\mu(U)\,UAU^\dagger = \frac{\mathbb{1}\,\mathrm{Tr}[A]}{2^n} \tag{24}$$

$$\mathbb{E}_U[AUBU^\dagger CUDU^\dagger] = \frac{\mathrm{Tr}[BD]\,\mathrm{Tr}[C]A + \mathrm{Tr}[B]\,\mathrm{Tr}[D]AC}{2^{2n}-1} \tag{25}$$

$$-\frac{\mathrm{Tr}[BD]AC + \mathrm{Tr}[B]\,\mathrm{Tr}[C]\,\mathrm{Tr}[D]A}{2^n(2^{2n}-1)} \tag{26}$$

Statistics of the Hessian

Let $f(\boldsymbol{\theta}) = \mathrm{Tr}\big[OU(\boldsymbol{\theta})\,|0\rangle\langle0|\,U(\boldsymbol{\theta})^\dagger\big]$ and assume that the observable O is such that $\mathrm{Tr}[O] = 0$ and $\mathrm{Tr}\big[O^2\big] = 2^n$, as is the case of measuring a Pauli string. As shown in Eq. (19), diagonal elements of the Hessian matrix H can be calculated as

$$H_{ii} = \frac{\partial^2 f(\boldsymbol{\theta})}{\partial\theta_i^2} = \frac{1}{2}[f(\boldsymbol{\theta}+\pi\boldsymbol{e}_i) - f(\boldsymbol{\theta})]\,. \tag{27}$$

For simplicity, from now on we drop the explicit dependence on the parameter vector $\boldsymbol{\theta}$ when not explicitly needed. The variational parameters enter the quantum circuit via Pauli rotations $e^{-i\theta_i P_i/2}$ with $P_i = P_i^\dagger$ and $P_i^2 = \mathbb{1}$, and so the shifted unitary $U(\boldsymbol{\theta}+\pi\boldsymbol{e}_i)$ can be rewritten as

$$U(\boldsymbol{\theta}+\pi\boldsymbol{e}_i) = U_L e^{-i\pi P_i/2} U_R = -i\,U_L P_i U_R\,, \tag{28}$$

where U_L and U_R form a bipartition of the circuit at the position of the shifted angle, so that $U(\boldsymbol{\theta}) = U_L U_R$.

Assuming that the set of unitaries $\mathbb{U}_L$ generated by U_L is at least a 1-design, one has that

$$\mathbb{E}_{U_L}[f(\boldsymbol{\theta}+\pi\boldsymbol{e}_i)] = \mathbb{E}_{U_L}\Big[\mathrm{Tr}\Big[O\,U_L P_i U_R\,|0\rangle\langle0|\,U_R^\dagger P_i U_L^\dagger\Big]\Big] \tag{29}$$

$$= \mathrm{Tr}\Big[O\,\mathbb{E}_{U_L}\Big[U_L P_i U_R\,|0\rangle\langle0|\,U_R^\dagger P_i U_L^\dagger\Big]\Big] \tag{30}$$

$$= \mathrm{Tr}\left[O\,\frac{\mathrm{Tr}\Big[P_i U_R\,|0\rangle\langle0|\,U_R^\dagger P_i\Big]\mathbb{1}}{2^n}\right] = \frac{\mathrm{Tr}[O]}{2^n} = 0\,, \tag{31}$$

where in the first line we exchanged the trace and the expectation value since both are linear operations, and in the second line we made use of Eq. (24) for the first moment of the Haar distribution. Similarly, one can show that if $\mathbb{U}_R$ forms a

1-design, then averaging over it yields the same result, namely $\mathbb{E}_{U_R}[f(\boldsymbol{\theta} + \pi \boldsymbol{e}_i)] = 0$. The same calculation for $f(\boldsymbol{\theta})$ shows that $\mathbb{E}_{U_R}[f(\boldsymbol{\theta})] = \mathbb{E}_{U_L}[f(\boldsymbol{\theta})] = 0$.

Thus, for every diagonal element of the Hessian, if either $\mathbb{U}_L$ or $\mathbb{U}_{\mathbb{R}}$ is a 1-design (that is Eq. (24) hold), then its expectation value vanishes

$$\mathbb{E}_{U_R, U_L}[H_{ii}] = 0 \quad \forall i \quad \text{if either } \mathbb{U}_L \text{ or } \mathbb{U}_{\mathbb{R}} \text{ is a 1-design.} \tag{32}$$

The variance of the diagonal elements can be calculated in a similar manner, even though the calculation is more involved. Substituting Eq. (27) in the defition of the variance, one obtains

$$
\begin{aligned}
\mathrm{Var}[H_{ii}] &:= \mathbb{E}[H_{ii}^2] - \mathbb{E}[H_{ii}]^2 = \mathbb{E}[H_{ii}^2] \\
&= \frac{1}{4}\left[\mathbb{E}[f(\boldsymbol{\theta} + \pi \boldsymbol{e}_i)^2] + \mathbb{E}[f(\boldsymbol{\theta})^2] - 2\mathbb{E}[f(\boldsymbol{\theta} + \pi \boldsymbol{e}_i)f(\boldsymbol{\theta})] \right].
\end{aligned}
\tag{33}
$$

In order to use Eq. (26) for second moment integrals, we can rewrite these expectation values as follows

$$
\begin{aligned}
\mathbb{E}[f(\boldsymbol{\theta} + \pi \boldsymbol{e}_i)^2] &= \mathbb{E}\left[\mathrm{Tr}\left[O\, U_L P_i U_R \,|0\rangle\langle 0|\, U_R^\dagger P_i U_L^\dagger \right]^2 \right] \\
&= \mathbb{E}\left[\mathrm{Tr}\left[O\, U_L P_i U_R \,|0\rangle\langle 0|\, U_R^\dagger P_i U_L^\dagger \right] \langle 0| U_R^\dagger P_i U_L^\dagger O U_L P_i U_R |0\rangle \right] \\
&= \mathbb{E}\left[\mathrm{Tr}\left[O\, U_L P_i U_R \,|0\rangle\langle 0|\, U_R^\dagger P_i U_L^\dagger O U_L P_i U_R \,|0\rangle\langle 0|\, U_R^\dagger P_i U_L^\dagger \right] \right] \\
&= \mathrm{Tr}\left[\mathbb{E}[O\, U_L P_i U_R \,|0\rangle\langle 0|\, U_R^\dagger P_i U_L^\dagger O U_L P_i U_R \,|0\rangle\langle 0|\, U_R^\dagger P_i U_L^\dagger] \right], \quad (34)
\end{aligned}
$$

and similarly for the remaining two terms. Assuming that the set of unitaries $\mathbb{U}_L$ generated by U_L is a 2-design, then

$$
\mathbb{E}_{U_L}[f(\boldsymbol{\theta} + \pi \boldsymbol{e}_i)^2] = \mathrm{Tr}\left[\mathbb{E}_{U_L}[O\, U_L \underbrace{P_i U_R \,|0\rangle\langle 0|\, U_R^\dagger P_i}_{B}\, U_L^\dagger O U_L \underbrace{P_i U_R \,|0\rangle\langle 0|\, U_R^\dagger P_i}_{B}\, U_L^\dagger] \right]
\tag{35}
$$

$$
= \mathrm{Tr}\left[\frac{\mathrm{Tr}[B^2]\,\mathrm{Tr}[O]O + \mathrm{Tr}[B]^2 O^2}{2^{2n} - 1} - \frac{\mathrm{Tr}[B^2]O^2 + \mathrm{Tr}[B]^2\,\mathrm{Tr}[O]O}{2^n(2^{2n} - 1)} \right]
\tag{36}
$$

$$
= \frac{\mathrm{Tr}[O]^2 + \mathrm{Tr}[O^2]}{2^{2n} - 1} - \frac{\mathrm{Tr}[O^2] + \mathrm{Tr}[O]^2}{2^n(2^{2n} - 1)} = \frac{1}{2^n + 1},
\tag{37}
$$

where in the second line we made use of Eq. (26), and the third line the used that $\mathrm{Tr}[B] = \mathrm{Tr}[B^2] = 1$ since $B = P_i U_R \,|0\rangle\langle 0|\, U_R^\dagger P_i$ is a projector, and that $\mathrm{Tr}[O] = 0$

and $\text{Tr}[O^2] = 2^n$. Similarly, one can show that integration over $\mathbb{U}_R$ yields the same result. Also, the same calculation leads to $\mathbb{E}_{U_L}[f(\boldsymbol{\theta})^2] = \mathbb{E}_{U_R}[f(\boldsymbol{\theta})^2] = 1/(2^n + 1)$. Thus, if either $\mathbb{U}_L$ or $\mathbb{U}_\mathbb{R}$ is a 2-design then

$$\mathbb{E}_{U_R, U_L}[f(\boldsymbol{\theta})^2] = \mathbb{E}_{U_R, U_L}[f(\boldsymbol{\theta} + \pi\boldsymbol{e}_i)^2] = \frac{1}{2^n + 1} \quad \forall i \quad \text{if either } \mathbb{U}_L \text{ or } \mathbb{U}_\mathbb{R} \text{ is a 2-design.}$$
(38)

Now we evaluate the correlation term $\mathbb{E}[f(\boldsymbol{\theta} + \pi\boldsymbol{e}_i)f(\boldsymbol{\theta})]$. If $\mathbb{U}_L$ is a 2-design, then

$$\mathbb{E}_{U_L}[f(\boldsymbol{\theta} + \pi\boldsymbol{e}_i)f(\boldsymbol{\theta})] = \text{Tr}\left[\mathbb{E}_{U_L}\left[O\,U_L P_i U_R \, |0\rangle\langle0| \, U_R^\dagger U_L^\dagger O U_L U_R \, |0\rangle\langle0| \, U_R^\dagger P_i U_L^\dagger\right]\right]$$

$$= \text{Tr}\left[\frac{\text{Tr}\left[P_i U_R \, |0\rangle\langle0| \, U_R^\dagger\right]^2 O^2}{2^{2n} - 1} - \frac{O^2}{2^n(2^{2n} - 1)}\right]$$

$$= \frac{1}{2^{2n} - 1}\left[2^n \, \text{Tr}\left[P_i U_R \, |0\rangle\langle0| \, U_R^\dagger\right]^2 - 1\right].$$
(39)

While if $\mathbb{U}_R$ is a 2-design instead it holds

$$\mathbb{E}_{U_R}[f(\boldsymbol{\theta} + \pi\boldsymbol{e}_i)f(\boldsymbol{\theta})] = \text{Tr}\left[O\,U_L P_i \, \mathbb{E}_{U_R}\left[U_R \, |0\rangle\langle0| \, U_R^\dagger U_L^\dagger O U_L U_R \, |0\rangle\langle0| \, U_R^\dagger\right] P_i U_L^\dagger\right]$$

$$= \text{Tr}\left[O\,U_L P_i \, \frac{(2^n - 1) U_L^\dagger O U_L}{2^n(2^{2n} - 1)} \, P_i U_L^\dagger\right]$$

$$= \frac{1}{2^n(2^n + 1)} \, \text{Tr}\left[O\,U_L P_i U_L^\dagger O U_L P_i U_L^\dagger\right].$$
(40)

If both of them are 2-designs, then continuing from Eq. (40), one obtains

$$\mathbb{E}_{U_L, U_R}[f(\boldsymbol{\theta} + \pi\boldsymbol{e}_i)f(\boldsymbol{\theta})] = \frac{1}{2^n(2^n + 1)} \, \text{Tr}\left[\mathbb{E}_{U_L}\left[O\,U_L P_i U_L^\dagger O U_L P_i U_L^\dagger\right]\right]$$

$$= \frac{1}{2^n(2^n + 1)} \, \text{Tr}\left[\frac{\text{Tr}[P_i]^2 O^2 + \text{Tr}[P_i^2]\,\text{Tr}[O]O}{2^{2n} - 1} - \frac{\text{Tr}[P_i^2]O^2 + \text{Tr}[P_i]^2\,\text{Tr}[O]O}{2^n(2^{2n} - 1)}\right]$$

$$= -\frac{1}{2^n(2^n + 1)} \frac{\text{Tr}[P_i^2]\,\text{Tr}[O^2]}{2^n(2^{2n} - 1)} = -\frac{1}{(2^n + 1)(2^{2n} - 1)} \in \mathcal{O}(2^{-3n})$$
(41)

Finally, plugging Eqs. (39), (40) and (41) in Eq. (33), one has $\forall i = 1, \ldots, M$

$$\mathrm{Var}_{U_L, U_R}[H_{ii}] = \frac{1}{2}\mathbb{E}[f(\boldsymbol{\theta})^2] - \frac{1}{2}\mathbb{E}[f(\boldsymbol{\theta} + \pi \boldsymbol{e}_i)f(\boldsymbol{\theta})]$$

$$= \frac{1}{2(2^n + 1)} - \frac{1}{2}\begin{cases} \dfrac{1}{2^{2n} - 1}\left[2^n \,\mathrm{Tr}\left[P_i U_R \,|0\rangle\langle 0|\, U_R^\dagger\right]^2 - 1\right] & \forall i\,, \text{if } \mathbb{U}_L \text{ 2-design} \\[4mm] \dfrac{1}{2^n(2^n + 1)}\,\mathrm{Tr}\left[O\,U_L P_i U_L^\dagger O U_L P_i U_L^\dagger\right] & \forall i\,, \text{if } \mathbb{U}_R \text{ 2-design} \\[4mm] -\dfrac{1}{(2^n + 1)(2^{2n} - 1)} & \forall i\,, \text{if } \mathbb{U}_L, \mathbb{U}_R \text{ 2-designs} \end{cases}$$

$$(42)$$

where $\mathbb{U}_R = \mathbb{U}_R^{(i)}$ and $\mathbb{U}_L = \mathbb{U}_L^{(i)}$ are defined as in Eq. (28) and actually depend on the index i of the parameter.

Not surprisingly, as it happens for first order derivatives, also second order derivatives of PQCs are found to be exponentially vanishing [51, 48], as from Eq. (42) one can check that $\mathrm{Var}[H_{ii}] \in \mathcal{O}(2^{-n})$.

Statistics of the trace of the Hessian

The average value of the trace of the Hessian is easily found to be zero using Eq. (32), in fact

$$\mathbb{E}_{U_R, U_L}[\mathrm{Tr}[H]] = \sum_{i=1}^{M} \mathbb{E}_{U_R^{(i)}, U_L^{(i)}}[H_{ii}] = 0\,, \qquad (43)$$

where we assume that for every parameter i either $\mathbb{U}_R^{(i)}$ or $\mathbb{U}_L^{(i)}$ is a 1-design. The variance of the trace is instead

$$\mathrm{Var}_{U_R, U_L}[\mathrm{Tr}[H]] = \mathrm{Var}\left[\sum_{i=1}^{M} H_{ii}\right] = \sum_{i=1}^{M} \mathrm{Var}[H_{ii}] + 2\sum_{i<j}^{M} \mathrm{Cov}[H_{ii}H_{jj}]\,. \qquad (44)$$

We can upper bound this quantity using the covariance inequality [308],

$$|\mathrm{Cov}[H_{ii}, H_{jj}]| \leq \sqrt{\mathrm{Var}[H_{ii}]\,\mathrm{Var}[H_{jj}]} \approx \mathrm{Var}[H_{ii}]\,,$$

were we assumed that $\mathrm{Var}[H_{ii}] \approx \mathrm{Var}[H_{jj}]\,\forall i, j$. Using that $\mathrm{Var}[H_{ii}] \in \mathcal{O}(2^{-n})$ one finally has

$$\mathrm{Var}_{U_R, U_L}[\mathrm{Tr}[H]] \leq \sum_{i=1}^{M} \mathrm{Var}[H_{ii}] + 2\sum_{i<j}^{M} \mathrm{Var}[H_{ii}] \in \mathcal{O}\left(\frac{M^2}{2^n}\right)\,. \qquad (45)$$

Alternatively, one can obtain a tighter yet qualitative approximation by explicitly considering the nature of the sums in Eq. (44). First, by using Eq. (27), the covariance term is explicitly

$$
\begin{aligned}
\mathrm{Cov}[H_{ii}, H_{jj}] &= \mathbb{E}[H_{ii}H_{jj}] \\
&= \frac{1}{4}\mathbb{E}[(f_i - f)(f_j - f)] \\
&= \frac{1}{4}\mathbb{E}[f^2] + \frac{1}{4}\mathbb{E}[f_i f_j] - \frac{1}{4}\mathbb{E}[f_i f] - \frac{1}{4}\mathbb{E}[f_j f],
\end{aligned}
\tag{46}
$$

where for ease of notation we defined $f_{i,j} = f(\boldsymbol{\theta} + \pi \boldsymbol{e}_{i,j})$ and $f = f(\boldsymbol{\theta})$. Note that except for the first term which is always positive, all remaining correlations terms can be both positive and negative. Also, all of these terms are bounded from above by the same quantity, as via Cauchy-Schwarz it follows

$$
|\mathbb{E}[f_i f_j]| \leq \sqrt{\mathbb{E}[f_i^2]\mathbb{E}[f_j^2]} = \frac{1}{2^n + 1} \quad \text{and} \quad |\mathbb{E}[f_i f]| \leq \sqrt{\mathbb{E}[f_i^2]\mathbb{E}[f^2]} = \frac{1}{2^n + 1},
\tag{47}
$$

where we have used $E[f^2] = E[f_i^2] = 1/(2^n + 1)$ from Eq. (38). Then, the variance can be written as

$$
\begin{aligned}
\mathrm{Var}_{U_R, U_L}[\mathrm{Tr}[H]] &= \sum_{i=1}^{M} \mathrm{Var}[H_{ii}] + 2\sum_{i<j}^{M} \mathbb{E}[H_{ii}H_{jj}] \\
&= \sum_{i=1}^{M} \frac{\mathbb{E}[f^2] - \mathbb{E}[f_i f]}{2} + 2\sum_{i<j}^{M} \frac{\mathbb{E}[f^2] + \mathbb{E}[f_i f_j] - \mathbb{E}[f_i f] - \mathbb{E}[f_j f]}{4} \\
&= \frac{1}{2}\left(\sum_{i=1}^{M} + \sum_{i<j}^{M}\right)\mathbb{E}[f^2] - \frac{1}{2}\left(\sum_{i=1}^{M}\mathbb{E}[f_i f] + \sum_{i<j}^{M}\mathbb{E}[f_i f] + \sum_{i<j}^{M}\mathbb{E}[f_j f]\right) + \frac{1}{2}\sum_{i<j}^{M}\mathbb{E}[f_i f_j] \\
&= \frac{M(M+1)}{4}\mathbb{E}[f^2] \underbrace{- \frac{M}{2}\sum_{i=1}^{M}\mathbb{E}[f_i f] + \frac{1}{2}\sum_{i<j}^{M}\mathbb{E}[f_i f_j]}_{\Delta}.
\end{aligned}
\tag{48}
$$

Numerical simulations In addition to Figure 7.6 in the main text, in Figure 5 we report numerical evidence for the trace of the Hessian for two common hardware-efficient parametrized quantum circuit ansatzes. The histograms represent the frequency of obtaining a given value of the trace of the Hessian $\mathrm{Tr}[H(\boldsymbol{\theta})]$ upon random assignments of the parameters. The length of the arrows are, respectively: "Numerical 2σ" (black solid line) twice the statistical standard deviation computed from the numerical results, "Approximation" (dashed red) twice the square root of
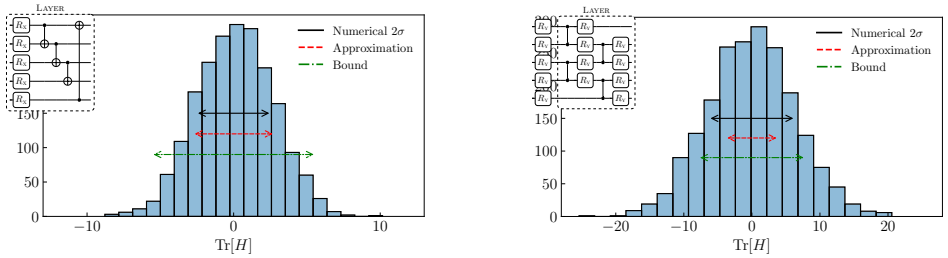
Figure 5: Simulation results of evaluating the trace of the Hessian matrix for two different hardware-efficient ansatzes with random values of the parameters. The plot on the left is obtained using the layer template shown in the figure for $n = 6$ qubits and $l = 6$ layers. The plot on the right instead with $n = 5$ and $l = 5$ layers of the template shown in the corresponding inset. The simulations are performed by sampling 2000 random parameter vectors $\boldsymbol{\theta}_m$ with $\theta_i \sim \text{Unif}[0, 2\pi[$, evaluating the trace of the Hessian matrix $\text{Tr}[H(\boldsymbol{\theta})]$, and then building the histogram to show its frequency distribution. In both experiments the measured observable is $Z^{\otimes n}$. The length of the arrows are respectively: "Numerical 2σ" (black solid line) twice the numerical standard deviation, "Approximation" (dashed red) twice the square root of the approximation in Eq. (49), "Bound" (dashed-dotted green) twice the square root of the upper Bound in Eq. (45). These parametrized circuits correspond to the templates `BasicEntanglinLayer` and `Simplified2Design` defined in Pennylane [**?**], and used for example in [44] to study barren plateaus.

the Eq. (48) with $\Delta = 0$, "Bound" (dashed-dotted green) twice the square root of the upper Bound in Eq. (45).

All simulations confirm the bound (45), and, more interestingly, both the circuit on the left of Fig. 5 and the one in Fig. 7.6 in the main text, have a numerical variance which is very well approximated by Eq. (48) with $\Delta = 0$. We conjecture this is due to the fact that all correlation terms in Eq. (48) are roughly of the same order of magnitude (see Eq. (47)), and can be either positive and negative, depending on the parameter and the specifics of the ansatz. Thus, one can expect the whole contribution to either vanish $\Delta \approx 0$, or be negligible with respect to the leading term. If this is the case, then substituting $\mathbb{E}[f^2] = 1/(2^n + 1)$, the variance of the Hessian is approximately

$$\text{Var}_{U_R, U_L}[\text{Tr}[H]] \approx \frac{M(M+1)}{4}\mathbb{E}[f^2] = \frac{M(M+1)}{4(2^n + 1)} \approx \frac{1}{4}\frac{M^2}{2^n} \,, \qquad (49)$$

which is four times smaller then the upper bound Eq. (45), but clearly has the same scaling. While we numerically verified it also at other number of qubits, more investigations are needed to understand if and when this approximation holds, and we leave a detailed study of this phenomenon for future work.

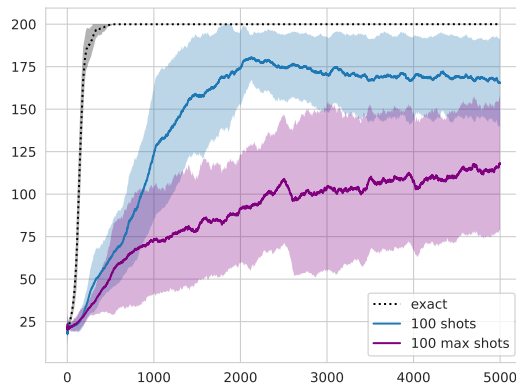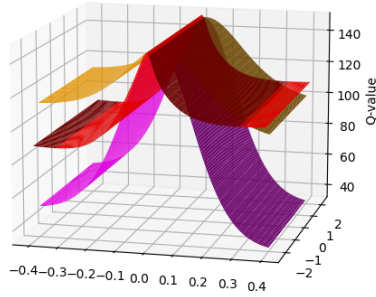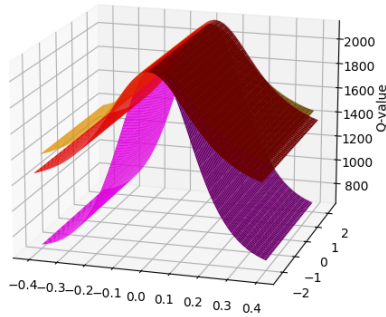# Additional results for flexible vs. fixed number of shots in Q-learning

Figure 6: Performance of agents trained with a fixed number of 100 shots (blue) and $m_{\max} = 100$ with flexible shot allocation (purple), compared to model trained without shot noise (black dotted curve).

Visualization of CartPole policies obtained with Q-learning

(a) $\sigma = 0$

(b) $\sigma = 0.2$

Figure 7: Visualization of the Q-functions learned in the noise-free (a) and noisy (b) settings. The red surface shows Q-values for pole angle and cart position, orange for pole angle and cart velocity, and magenta for pole angle and pole velocity.

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