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Classical shadows with Pauli-invariant unitary ensembles

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Classical shadows provide a noise-resilient and sample-efficient method for learning quantum system properties, relying on a user-specified unitary ensemble. What is the weakest assumption on this ensemble that can still yield meaningful results? To address this, we focus on Pauli-invariant unitary ensembles—those invariant under multiplication by Pauli operators. For these ensembles, we present explicit formulas for the reconstruction map and sample complexity bounds and extend our results to the case when noise impacts the protocol implementation. Two applications are explored: one for locally scrambled unitary ensembles, where we present formulas for the reconstruction map and sample complexity bounds that circumvent the need to solve an exponential-sized linear system, and another for the classical shadows of quantum channels. Our results establish a unified framework for classical shadows with Pauli-invariant unitary ensembles, applicable to both noisy and noiseless scenarios for states and channels and primed for implementation on near-term quantum devices.

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INTRODUCTION

Learning the properties of an unknown but physically accessible quantum system is a fundamental task in quantum information processing^{1–3}. A standard tool for this task is quantum tomography, a process by which one recovers a classical description of a quantum system through performing measurements on it. Unfortunately, finding the full description of a quantum system by quantum tomography is computationally intensive; it requires an exponential number of copies of the system^{4–6}.

Recently, Huang, Kueng, and Preskill introduced a novel method—the classical shadow paradigm¹—to circumvent the above limitation. A key insight behind classical shadows rests on the fact that in many cases one does not need to learn a complete description of a quantum system; one can learn its most useful properties from a minimal sketch of the quantum system, the classical shadow. The classical shadow paradigm, with the sample efficiency it touts, has attracted considerable attention over the last couple of years⁷. Several applications have been proposed^{1,8–21}, ranging from the estimation of properties of quantum states and gates to quantum chaos in quantum evolution. Moreover, several improved versions of this protocol have been developed^{1,8,22–36}, such as noise-resilient versions^{20,37}.

The performance of the classical shadow protocol depends on several factors. In particular, it depends on an ensemble of unitary operators from which an operation is chosen randomly to be applied to the unknown quantum state. A user must choose this ensemble in advance, according to some desiderata, such as the need for the shadow channel to be invertible and for one to have an efficient algorithm for sampling a unitary from the ensemble. Several unitary ensembles have been considered by previous authors, including the local and global Clifford ensembles¹, fermionic Gaussian unitaries²⁸, chaotic Hamiltonian evolutions²⁷, locally scrambled unitary ensembles²⁶ and other short-depth quantum circuits. One motivation for studying short-depth quantum circuits is that random unitaries based on these random circuits could be more powerful in predicting properties of quantum systems³⁸ than the original proposals.

One can ask: what is the weakest assumption on the unitary ensemble that would still yield universal, meaningful and interesting results? Our candidate solution to this question is the assumption that the unitary ensemble is invariant under multiplication by a Pauli operator. Ensembles satisfying this assumption—namely the Pauli-invariant unitary ensembles—include a wide range of ensembles, including the Pauli group, the local and global Clifford groups, locally scrambled unitary ensembles, and short-depth 2-qubit Clifford circuits. The goal of this work is to provide a unified framework for the classical shadow protocol with Pauli-invariant unitary ensembles in both the noiseless and noisy settings.

The rest of our paper is structured as follows. In Section (“General framework for Pauli-invariant unitary ensembles”), we introduce the framework of classical shadows with Pauli-invariant unitary ensembles and provide an explicit formula for the shadow channel and reconstruction map, which are key elements in the classical shadow protocol described in Section (“Preliminaries: Classical shadows”). In addition, we establish a connection between the reconstruction map and the entanglement features of the dynamics. We give upper bounds on the sample complexity in terms of the average shadow norm for the task of expectation estimation using the classical shadow protocol. Considering the fact that noise is inevitable in the noisy intermediate-scale quantum (NISQ) era, we consider classical shadows for Pauli-invariant unitary ensembles in the presence of noise in Section (“Classical shadows with noise”). This generalizes our results from the noiseless case to the noisy case.

In Sections (“Application to locally scrambled unitary ensembles”) and (“Application to quantum channels”), we provide two applications of our main results. First, we investigate locally scrambled unitary ensembles, which are a special example of Pauli-invariant unitary ensembles. We provide an explicit reconstruction map, addressing a crucial gap in a previous approach provided by²⁶, which specifies the map only in terms of a solution of an exponential-sized system of linear equations; by contrast, using our explicit formula, ours circumvents the need to solve such an exponential-sized linear system. Second, we apply our results to the shadow process tomography of quantum channels using the Choi-Jamiołkowski isomorphism, thereby generalizing

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the results of refs. 29,30 to the broad class of Pauli-invariant unitary ensembles.

RESULTS

Preliminaries: classical shadows

Let us begin by describing the classical shadow protocol that was introduced in ref. 1. A user will have to pre-decide on a unitary ensemble $\mathcal{E} = \{(U, P(U))\}_{U \in \mathcal{U}}$, where \mathcal{U} is a set of unitary operators and P is a probability distribution on \mathcal{U} . The first step is choosing a random unitary U from the unitary ensemble \mathcal{E} according to the specified distribution $P(U)$. The unitary U is then applied to ρ and a computational basis measurement is performed on the resultant state to obtain an n -bit string $\vec{b} = b_1 b_2 \dots b_n \in \{0, 1\}^n$. We construct the state

$$\hat{\sigma}_{U, \vec{b}} = U^\dagger |\vec{b}\rangle \langle \vec{b}| U, \quad (1)$$

which is stored in classical memory. Note that this produces an ensemble of states

$$\mathcal{E}_\rho = \left\{ \left(\hat{\sigma}_{U, \vec{b}}, P(U, \vec{b}) \right) \right\}_{U, \vec{b}}, \quad (2)$$

where $P(U, \vec{b}) = P(U)P(\vec{b}|U)$ and $P(\vec{b}|U) = \text{Tr}[\hat{\sigma}_{U, \vec{b}} \rho]$. The expected value of this ensemble is given by

$$\sigma = \mathbb{E}_{\hat{\sigma} \in \mathcal{E}_\rho} \hat{\sigma} = \mathbb{E}_U \sum_{\vec{b}} \hat{\sigma}_{U, \vec{b}} \text{Tr} \left[\hat{\sigma}_{U, \vec{b}} \rho \right] := \mathcal{M}[\rho], \quad (3)$$

where \mathcal{M} —called the shadow channel—is a completely positive and trace-preserving map. To construct the classical shadow, the shadow channel needs to be invertible. If the conditions for invertibility are met, the inverse of the shadow channel \mathcal{M}^{-1} , called the reconstruction map, is applied to the classically stored $\hat{\sigma}_{U, \vec{b}}$ to obtain the classical snapshot $\hat{\rho} = \mathcal{M}^{-1}[\hat{\sigma}_{U, \vec{b}}]$, which is called the classical shadow. As required, $\hat{\rho}$ is an unbiased estimator of ρ :

$$\rho = \mathcal{M}^{-1}[\sigma] = \mathbb{E}_{\hat{\sigma} \in \mathcal{E}_\rho} \mathcal{M}^{-1}[\hat{\sigma}] = \mathbb{E}_{U, \vec{b}} \mathcal{M}^{-1}(\hat{\sigma}_{U, \vec{b}}) = \mathbb{E}_{U, \vec{b}} [\hat{\rho}]. \quad (4)$$

As illustrated above, the reconstruction map \mathcal{M}^{-1} plays a pivotal role in the classical shadow protocol. However, for arbitrary unitary ensembles, no general closed-form analytic formula is known for \mathcal{M}^{-1} . Instead, prior to this study, it was only for a handful of unitary ensembles (e.g., the local and global Clifford ensembles) that analytic expressions have been derived. In this study, we address this gap by presenting an explicit formula for the reconstruction map for the large class of Pauli-invariant unitary ensembles, thereby enlarging the class of ensembles for which such expressions are known.

General framework for Pauli-invariant unitary ensembles

In this paper, we consider classical shadows with Pauli-invariant unitary ensembles. We start by introducing these ensembles, before deriving our main results characterizing the performance of classical shadow protocols utilizing these ensembles.

We denote the set of Pauli operators on n qubits by $\mathcal{P}_n = \{P_{\vec{a}} = \otimes_i P_{a_i} : \vec{a} \in V^n\}$, where $V := \mathbb{Z}_2 \times \mathbb{Z}_2 = \{(0, 0), (0, 1), (1, 0), (1, 1)\}$, and $P_{(x, z)} = i^{xz} X^x Z^z$, i.e., $P_{(0,0)} = \mathbb{I}$, $P_{(0,1)} = Z$, $P_{(1,0)} = X$, $P_{(1,1)} = Y$. A given unitary ensemble $\mathcal{E} = \{(U, P(U))\}_{U \in \mathcal{U}}$ is called Pauli-invariant, if the probability distribution $P(U)$ satisfies the following (right) Pauli-invariant condition:

$$P(U) = P(UP_{\vec{a}}), \quad \forall P_{\vec{a}} \in \mathcal{P}_n. \quad (5)$$

This is a weak assumption, and many unitary ensembles satisfy this condition, for example, (1) the Pauli group $\{\pm 1, \pm i\} \times \mathcal{P}_n$; (2) D -dimensional local, random quantum circuits³⁹; (3) local Clifford unitaries; (4) global Clifford unitaries; and (5) short-depth 2-qubit Clifford circuits.

For Pauli-invariant unitary ensembles, we will now provide an explicit formula for the shadow channel \mathcal{M} and the corresponding reconstruction map \mathcal{M}^{-1} , if it exists. The key idea is to use the Pauli coefficients in the decomposition in terms of Pauli operators, noting that the Pauli operators form an orthonormal basis with respect to the scaled Hilbert-Schmidt inner product $\langle A, B \rangle = \frac{1}{2^n} \text{Tr}[A^\dagger B]$ for an n -qubit system. These Pauli coefficients can be thought of as quantum Fourier coefficients, which have found extensive uses in a myriad of applications, including quantum Boolean functions⁴⁰, quantum circuit complexity⁴¹, quantum scrambling⁴² and quantum convolutions^{43–45}. For clarity of presentation, the detailed proofs of all the results in this section are provided in Supplementary Note 2. This follows Supplementary Note 1, which introduces the symplectic inner product used in these proofs.

Theorem 1. (Shadow channel and reconstruction map) For a Pauli-invariant unitary ensemble \mathcal{E} , the shadow channel can be written as

$$\mathcal{M}[\rho] = \frac{1}{2^n} \sum_{\vec{a} \in V^n} W_\mathcal{E}[\vec{a}] \text{Tr}[\rho P_{\vec{a}}] P_{\vec{a}}, \quad (6)$$

where $W_\mathcal{E}[\vec{a}]$ is the average squared Pauli coefficient of the classical shadow, defined as

$$W_\mathcal{E}[\vec{a}] = \mathbb{E}_{U, \vec{b}} W_{\hat{\sigma}_{U, \vec{b}}}[\vec{a}], \quad (7)$$

where $\mathbb{E}_{U, \vec{b}} := \frac{1}{2^n} \sum_{U, \vec{b}}$ denotes the average with respect to the uniform distribution over n -bit strings. For a state σ , we have used the notation $W_\sigma[\vec{a}] := |\text{Tr}[\sigma P_{\vec{a}}]|^2$ to denote the square of the \vec{a} -th Pauli coefficient of σ .

For Pauli-invariant unitary ensembles, the reconstruction map \mathcal{M}^{-1} exists if and only if $W_\mathcal{E}[\vec{a}] > 0$ for all \vec{a} . If it exists, the reconstruction map, which is diagonal in the Pauli basis, is completely specified by its action on the Pauli basis elements as follows:

$$\mathcal{M}^{-1}[P_{\vec{a}}] = W_\mathcal{E}[\vec{a}]^{-1} P_{\vec{a}}. \quad (8)$$

Now, let us discuss the connection between the coefficients of the reconstruction map $W_\mathcal{E}$ and the 2nd entanglement feature^{46,47}, which has been used to describe the entangling power of unitary ensembles and is defined as follows:

$$E_\mathcal{E}^{(2)}[A] = \mathbb{E}_U \mathbb{E}_{\vec{a}} e^{-S_A^{(2)}(\hat{\sigma}_{U, \vec{a}})}, \quad (9)$$

where A is a subset of $[n]$, $S_A^{(2)}(\sigma) = -\log \text{Tr}[\sigma_A^2]$ denotes the 2nd Rényi entanglement entropy of the state σ on the subset A , and $\sigma_A = \text{Tr}_{A^c}[\sigma]$. For any subset $S \subset [n]$, let us define $W_\mathcal{E}[S]$ as the sum of the coefficients whose support is S , i.e.,

$$W_\mathcal{E}[S] = \sum_{\vec{a}: \text{supp}(\vec{a})=S} W_\mathcal{E}[\vec{a}], \quad (10)$$

where $\text{supp}(\vec{a})$ denotes the support of the vector \vec{a} . The following proposition expresses $W_\mathcal{E}[S]$ in terms of the 2nd entanglement feature.

Proposition 2. (Connection with entanglement feature for Pauli-invariant unitary ensemble) The coefficients of the

reconstruction map can be expressed as follows:

$$W_{\mathcal{E}}[S] = (-1)^{|S|} \sum_{A \subset S} (-2)^{|A|} E_{\mathcal{E}}^{(2)}[A]. \quad (11)$$

Now, let us consider the sample complexity for the task of expectation estimation using classical shadows with Pauli-invariant unitary ensembles. We shall make use of the result from ref. ¹ that the sample complexity of classical shadows with the input state ρ and an observable O is upper bounded by the following (squared) shadow norm:

$$\|O\|_{\mathcal{E},\rho}^2 = \mathbb{E}_{\mathcal{E},\rho} \hat{\sigma}[\hat{\sigma}]^2, \quad (12)$$

where the estimator $\hat{\sigma}$ of the observable O is given by $\hat{\sigma} = \text{Tr}[O\mathcal{M}^{-1}[\hat{\sigma}]]$.

Lemma 3. (Huang et al.¹) The sample complexity \mathcal{S} needed to accurately predict a collection of N linear target functions $\{\text{Tr}[O_i\rho]\}_{i=1}^N$ with error ϵ and failure probability δ is

$$\mathcal{S} = O\left(\frac{\log(N/\delta)}{\epsilon^2} \max_{1 \leq i \leq N} \|O_i - \frac{1}{2^n} \text{Tr}[O_i] \mathbb{I}\|_{\mathcal{E},\rho}^2\right).$$

In general, the shadow norm is hard to compute, though for special cases, closed-form expressions for the shadow norm can be derived. To this end, let us consider the widely used Pauli operators O as observables. For this case, we provide a unified formula for the shadow norm corresponding to all Pauli-invariant unitary ensembles.

Proposition 4. (Shadow norm for Pauli-invariant unitary ensembles for Pauli observables) If the observable O is the Pauli operator $P_{\vec{a}}$, then the (squared) shadow norm for a Pauli-invariant unitary ensemble is equal to

$$\|P_{\vec{a}}\|_{\mathcal{E},\rho}^2 = W_{\mathcal{E}}[\vec{a}]^{-1}. \quad (13)$$

Hence the sample complexity is bounded above by

$$O\left(\frac{\log(N/\delta)}{\epsilon^2} W_{\mathcal{E}}[\vec{a}]^{-1}\right). \quad (14)$$

Note that the shadow norm $\|O\|_{\mathcal{E}}$ usually depends on the input state ρ . If we are interested in the expectation of the shadow norm over some unitary ensemble instead of some specific state, we will need a notion of an average shadow norm. To this end, let us consider the (squared) average shadow norm over the Pauli group, defined as $\|O\|_{\mathcal{E}}^2 = \mathbb{E}_{V \in \mathcal{P}_n} \|O\|_{\mathcal{E},\rho^V}^2$. The following proposition gives an expression for the average shadow norm.

Proposition 5. (Average shadow norm for Pauli-invariant unitary ensemble) The (squared) average shadow norm over the Pauli group $\|O\|_{\mathcal{E}}^2$ can be expressed as follows:

$$\|O\|_{\mathcal{E}}^2 = \frac{1}{4^n} \sum_{\vec{a} \in V^n} W_{\mathcal{E}}[\vec{a}]^{-1} W_O[\vec{a}], \quad (15)$$

where $W_O[\vec{a}] = |\text{Tr}[OP_{\vec{a}}]|^2$. Therefore, given a set of N traceless observables $\{O_i\}_{i=1}^N$, the average shadow norm provides the following lower bound for the sample complexity:

$$\mathcal{S} \geq \frac{\log(N/\delta)}{\epsilon^2} \max_{1 \leq i \leq N} \langle \vec{W}_{\mathcal{E}}^{-1}, \vec{W}_{O_i} \rangle, \quad (16)$$

where the (normalized) inner product is defined as $\langle \vec{W}_{\mathcal{E}}^{-1}, \vec{W}_{O_i} \rangle := \frac{1}{4^n} \sum_{\vec{a} \in V^n} W_{\mathcal{E}}[\vec{a}]^{-1} W_{O_i}[\vec{a}]$.

Classical shadows with noise

Considering the fact that noise is unavoidable in real-world experiments, it is necessary to employ error mitigation techniques to make classical shadows useful in the presence of noise. In this subsection, let us consider noisy classical shadows with a Pauli-invariant unitary ensemble. Similar to the setting in^{20,37,48}, we shall assume that a noise channel Λ acts on the pre-measurement state $U\rho U^\dagger$ just before the measurement is performed. Such an assumption is obeyed by gate-independent, time-stationary, and Markovian noise^{20,49}. Similar to the noiseless case (2), the ensemble of states is given by $\mathcal{E}_{\Lambda,\rho} = \left\{ \left(\hat{\sigma}_{U,\vec{b}}, P(U,\vec{b}) \right) \right\}_{U,\vec{b}}$,

where $P_{\Lambda}(\vec{b}|U) = \text{Tr}[\vec{b} \langle \vec{b} | \Lambda[U\rho U^\dagger]]$. Hence, by taking the average of the post-measurement states, we have $\sigma =$

$\mathbb{E}_U \sum_{\vec{b}} \hat{\sigma}_{U,\vec{b}} \text{Tr}[\vec{b} \langle \vec{b} | \Lambda[U\rho U^\dagger]] = \mathcal{M}_{\Lambda}[\rho]$, where \mathcal{M}_{Λ} is the noisy shadow channel, and $\rho = \mathcal{M}_{\Lambda}^{-1}[\sigma]$, where $\mathcal{M}_{\Lambda}^{-1}$ is the noisy reconstruction map. We will now provide an explicit form for the noisy reconstruction map $\mathcal{M}_{\Lambda}^{-1}$. For clarity of presentation, the detailed proofs of all the results in this subsection are provided in Supplementary Note 5.

Theorem 6. (Shadow channel and reconstruction map in noisy case) Given a Pauli-invariant unitary ensemble \mathcal{E} and a noise channel Λ , the noisy shadow channel is given by

$$\mathcal{M}_{\Lambda}[\rho] = \frac{1}{2^n} \sum_{\vec{a}} W_{\mathcal{E}_{\Lambda}}[\vec{a}] \text{Tr}[\rho P_{\vec{a}}] P_{\vec{a}}, \quad (17)$$

where $W_{\mathcal{E}_{\Lambda}}[\vec{a}]$ is the average Pauli coefficient of the noisy classical shadow, and is defined as

$$W_{\mathcal{E}_{\Lambda}}[\vec{a}] = \mathbb{E}_{\vec{b}} \mathbb{E}_U \text{Tr}[\hat{\sigma}_{U,\vec{b}} P_{\vec{a}}] \text{Tr}[U^\dagger \Lambda^\dagger[|\vec{b}\rangle\langle\vec{b}|] U P_{\vec{a}}]. \quad (18)$$

For the Pauli-invariant unitary ensemble, $\mathcal{M}_{\Lambda}^{-1}$ exists if and only if $W_{\mathcal{E}_{\Lambda}}[\vec{a}] > 0$ for all \vec{a} . If it exists, the reconstruction map is defined by

$$\mathcal{M}_{\Lambda}^{-1}[P_{\vec{a}}] = W_{\mathcal{E}_{\Lambda}}[\vec{a}]^{-1} P_{\vec{a}}. \quad (19)$$

Now, let us consider the sample complexity of the noisy classical shadow protocol. Similar to the noiseless case, the sample complexity of the noisy classical shadow with the input state ρ and observable O is upper bounded by the (squared) noisy shadow norm $\|O\|_{\mathcal{E}_{\Lambda},\rho}^2 = \mathbb{E}_{\hat{\sigma} \in \mathcal{E}_{\Lambda}} \hat{\sigma}[\hat{\sigma}]^2$, where the estimator of the observable is taken to be $\hat{\sigma} = \text{Tr}[O\mathcal{M}_{\Lambda}^{-1}[\hat{\sigma}]]$. Let us also define the (squared) average shadow norm over the Pauli group for the noisy classical shadow to be $\|O\|_{\mathcal{E}_{\Lambda}}^2 = \mathbb{E}_{V \in \mathcal{P}_n} \|O\|_{\mathcal{E}_{\Lambda},\rho^V}^2$.

Proposition 7. If the observable O is taken to be the Pauli operator $P_{\vec{a}}$, the shadow norm is equal to

$$\|P_{\vec{a}}\|_{\mathcal{E}_{\Lambda},\rho}^2 = W_{\mathcal{E}_{\Lambda}}[\vec{a}]^{-2} W_{\mathcal{E}_{\Lambda}}^u[\vec{a}], \quad (20)$$

where $W_{\mathcal{E}_{\Lambda}}^u[\vec{a}]$ is defined as

$$W_{\mathcal{E}_{\Lambda}}^u[\vec{a}] = \mathbb{E}_U \mathbb{E}_{\vec{b}} \left| \text{Tr}[P_{\vec{a}} \hat{\sigma}_{U,\vec{b}}] \right|^2 \text{Tr}[\vec{b} \langle \vec{b} | \Lambda[\mathbb{I}]]. \quad (21)$$

Hence, if Λ is unital, then $W_{\mathcal{E}_{\Lambda}}^u[\vec{a}] = W_{\mathcal{E}}[\vec{a}]$. Moreover, the average shadow norm in the noisy classical shadow protocol with the noise channel Λ can be expressed as follows

$$\|O\|_{\mathcal{E}_{\Lambda}}^2 = \frac{1}{4^n} \sum_{\vec{a}} W_{\mathcal{E}_{\Lambda}}[\vec{a}]^{-2} W_{\mathcal{E}}^u[\vec{a}] W_O[\vec{a}]. \quad (22)$$

Let us now provide an example of noisy classical shadows and demonstrate how the performance of the protocol depends on the noise rate.

Example 1. Let us consider the case where the noise channel is the global depolarizing channel, defined as $D_p[\cdot] = (1-p)[\cdot] + p \frac{\text{Tr}[\cdot]\mathbb{I}}{2^n}$. The coefficients of the shadow channel can be expressed as

$$W_{\mathcal{E}_{D_p}}[\vec{a}] = (1-p)^{1-\delta_{\vec{a},\vec{0}}} W_{\mathcal{E}}[\vec{a}], \quad (23)$$

and the shadow norm for a Pauli operator $P_{\vec{a}}$ obeys the following identity

$$\|P_{\vec{a}}\|_{\mathcal{E}_{D_p},\rho}^2 = (1-p)^{2\delta_{\vec{a},\vec{0}}} \|P_{\vec{a}}\|_{\mathcal{E},\rho}^2, \quad (24)$$

where $\delta_{\vec{a},\vec{0}}$ denotes the Kronecker delta function. Hence the sample complexity for any non-identity Pauli operator is bounded by

$$O\left(\frac{1}{(1-p)^2} \frac{\log(N/\delta)}{\epsilon^2} W_{\mathcal{E}}[\vec{a}]^{-1}\right). \quad (25)$$

From the above equation, we see that depolarizing noise increases the number of samples needed for expectation estimation, with an increase that is proportional to the noise rate.

Application to locally scrambled unitary ensembles

First, let us apply our results to locally scrambled unitary ensembles, which are a special case of Pauli-invariant unitary ensembles. A unitary ensemble is said to be locally scrambled²⁶ if the probability distribution $P(U)$ satisfies local basis invariance, that is,

$$P(U) = P(UV), \quad \forall \text{unitaries } V = V_1 \otimes \cdots \otimes V_n. \quad (26)$$

It is easy to see that the Pauli-invariance assumption is weaker than the locally scrambled assumption, as locally scrambled unitary ensembles are Pauli-invariant. Not all Pauli-invariant unitary ensembles are locally scrambled though—a counterexample is the Pauli group.

Classical shadows with locally scrambled unitary ensembles were previously considered in ref.²⁶. However, a crucial limitation of the results presented therein is that the reconstruction map was left specified in terms of the solution of a linear system of size $O(2^n)$ without any explicit formula given for the map. By contrast, for our study, since locally scrambled unitary ensembles are a special case of the Pauli-invariant unitary ensembles, we get as a consequence of Theorem 1 an explicit formula for the reconstruction map that circumvents the need to solve an exponential-sized linear system. Our next proposition makes this explicit. For clarity of presentation, the detailed proofs of all the results in this subsection are provided in Supplementary Note 3.

Proposition 8. Given a locally scrambled unitary ensemble \mathcal{E} , the shadow channel is

$$\mathcal{M}[\rho] = \frac{1}{2^n} \sum_{S \subseteq [n]} \overline{W}_{\mathcal{E}}[S] \sum_{\vec{a}: \text{supp}(\vec{a})=S} \text{Tr}[\rho P_{\vec{a}}] P_{\vec{a}},$$

where $\overline{W}_{\mathcal{E}}[S]$ is defined as $\overline{W}_{\mathcal{E}}[S] = \mathbb{E}_{\vec{a}: \text{supp}(\vec{a})=S} W_{\mathcal{E}}[\vec{a}]$, and the reconstruction map is given by

$$\mathcal{M}^{-1}[P_{\vec{a}}] = \overline{W}_{\mathcal{E}}[\text{supp}(\vec{a})]^{-1} P_{\vec{a}}.$$

Our expression for the reconstruction map above may be compared with that given in ref.²⁶, which expressed the reconstruction map as $\mathcal{M}^{-1}[\sigma] = \sum_{S \subseteq [n]} r_S D^S[\sigma]$, where D^S denotes the $|S|$ -fold Kronecker product of the single-qubit erasure channel $D[\cdot] = \text{Tr}[\cdot]\mathbb{I}/2$ with itself acting on all the qubits indexed by S , and

the coefficients r_S are given as the solution of a linear system whose coefficients are the entanglement features. In the next proposition, we find an explicit formula for r_S in terms of the coefficients $\overline{W}_{\mathcal{E}}[S]$.

Proposition 9. Given a reconstruction map written as $\mathcal{M}^{-1}[\sigma] = \sum_S r_S D^S[\sigma]$, the coefficients r_S can be expressed in terms of $\overline{W}_{\mathcal{E}}[A]$ as follows

$$r_S = \sum_{A \subseteq S} (-1)^{|S|-|A|} \overline{W}_{\mathcal{E}}[A^c]^{-1}, \quad (27)$$

where A^c denotes the complement of A in $[n]$.

Using Proposition 2 and the fact that $W_{\mathcal{E}}[S] = 3^{|S|} \overline{W}_{\mathcal{E}}[S]$, our next corollary shows how the coefficients r_S can be expressed in terms of the entanglement feature.

Corollary 10. Given a reconstruction map written as $\mathcal{M}^{-1}[\sigma] = \sum_S r_S D^S[\sigma]$, the coefficients r_S can be expressed as follows

$$r_S = (-1)^{n+|S|} \sum_{A \subseteq S} 3^{|A^c|} \left[\sum_{B \subseteq A^c} (-2)^{|B|} E_{\mathcal{E}}^{(2)}[B] \right]^{-1}. \quad (28)$$

For the locally scrambled unitary ensembles, the average (squared) shadow norm is defined in ref.²⁶ as $\|O\|_{\mathcal{E}}^2 = \mathbb{E}_{V \in U(2)^n} \|O\|_{\mathcal{E}_{V\rho V}}^2$, which provides a typical lower bound for the sample complexity of expectation estimation using classical shadows with locally scrambled unitary ensembles.

Just as we have provided an explicit formula for the reconstruction map in terms of the entanglement feature, so too can we provide an explicit formula for the shadow norm using the entanglement feature.

Proposition 11. Given a locally scrambled unitary ensemble \mathcal{E} , the (squared) average shadow norm is

$$\|O\|_{\mathcal{E}}^2 = \frac{1}{4^n} \sum_{S \subseteq [n]} \overline{W}_{\mathcal{E}}[S]^{-1} W_O[S], \quad (29)$$

where $W_O[S] = \sum_{\vec{a}: \text{supp}(\vec{a})=S} W_O[\vec{a}]$.

Based on Propositions 2 and 11, we can express the (squared) average shadow norm in terms of the entanglement feature as follows:

$$\|O\|_{\mathcal{E}}^2 = \frac{1}{4^n} \sum_{S \subseteq [n]} (-3)^{|S|} W_O[S] \left[\sum_{A \subseteq [S]} (-2)^{|A|} E_{\mathcal{E}}^{(2)}[A] \right]^{-1}. \quad (30)$$

In summary, this section saw an application of our results to classical shadows with locally scrambled unitary ensembles, where we obtained an explicit formula for the reconstruction map and the average shadow norm in terms of the entanglement features, thus circumventing the need to solve the exponential-sized system of linear equations in ref.²⁶. These explicit formulae may be helpful for the further analysis of the role of entanglement in the classical shadow protocol, which we shall leave for future work.

Application to quantum channels

The classical shadow paradigm was recently extended to the shadow tomography of quantum channels^{29,30}. In these works, the unitary ensembles considered were the local and global Clifford ensembles. In this study, we extend their results to the case of Pauli-invariant unitary ensembles. For clarity of presentation, the detailed proofs of all the results in this subsection are provided in Supplementary Note 4.

Next, we shall outline the procedure proposed in refs. 29,30 for constructing the classical shadows for quantum channels. The unitary ensembles used will be assumed to be Pauli-invariant.

- (1) Prepare $|\vec{b}_i\rangle$ with $\vec{b}_i \in \{0, 1\}^n$ chosen uniformly randomly.
- (2) Apply a unitary U_i chosen from the locally Pauli-invariant ensemble \mathcal{E}_i .
- (3) Apply the quantum channel \mathcal{T} .
- (4) Apply a unitary U chosen from the locally Pauli-invariant ensemble \mathcal{E}_o , where the unitary ensemble \mathcal{E}_o may be different from \mathcal{E}_i .
- (5) Measure in the Pauli Z basis to get the output $\vec{b}_o \in \{0, 1\}^n$.

The post-measurement state is given by $\hat{\sigma}_{i,o} = U_i^\dagger |\vec{b}_i\rangle \langle \vec{b}_i| U_i \otimes U_o^\dagger |\vec{b}_o\rangle \langle \vec{b}_o| U_o$. Hence, given \vec{b}_i, U_i, U_o , the probability of getting the outcome \vec{b}_o is given by $P(\vec{b}_o | \vec{b}_i, U_i, U_o) = 2^n \text{Tr}[\hat{\sigma}_{i,o} \mathcal{J}(\mathcal{T})]$, where $\mathcal{J}(\mathcal{T}) = \mathbb{I} \otimes \mathcal{T}(|\Psi\rangle\langle\Psi|)$ is the Choi-Jamiolkowski state of \mathcal{T} , where $|\Psi\rangle = \frac{1}{\sqrt{2^n}} \sum_{\vec{i}} |\vec{i}\rangle |\vec{i}\rangle$ is the Bell state. It is easy to verify that $\sum_{\vec{b}_o} P(\vec{b}_o | \vec{b}_i, U_i, U_o) = 1$. Also, the probability of obtaining \vec{b}_i, U_i, U_o is equal to $P(\vec{b}_i, U_i, U_o) = P(\vec{b}_i)P(U_i)P(U_o)$. Hence, the ensemble of states is described by

$$\mathcal{E}_{i,o} = \{(\hat{\sigma}_{i,o}, P(\vec{b}_i, U_i, U_o, \vec{b}_o))\}, \quad (31)$$

where $P(\vec{b}_i, U_i, U_o, \vec{b}_o) := P(\vec{b}_i, U_i, U_o)P(\vec{b}_o | \vec{b}_i, U_i, U_o)$. Taking the average of the classical shadow, we obtain $\sigma = \mathbb{E}_{\hat{\sigma}_{i,o} \in \mathcal{E}_{i,o}} \hat{\sigma} = \mathcal{M}_{i,o}[\mathcal{J}(\mathcal{T})]$. To implement classical shadow tomography, the inverse of the shadow channel $\mathcal{M}_{i,o}^{-1}$ would need to be implemented. If the inverse exists, then $\mathcal{J}(\mathcal{T}) = \mathcal{M}_{i,o}^{-1}[\sigma] = \mathbb{E}_{\hat{\sigma}_{i,o} \in \mathcal{E}_{i,o}} \mathcal{M}_{i,o}^{-1}[\hat{\sigma}]$. Given a quantum state ρ and an observable O , the estimator $\hat{\sigma}$ is defined as $\hat{\sigma} = \text{Tr}[\mathcal{M}_{i,o}^{-1}[\hat{\sigma}_{i,o}]\rho^T \otimes O]$. Therefore, $\mathbb{E}[\hat{\sigma}] = \text{Tr}[\mathcal{T}[\rho]O]$.

Proposition 12. Given two Pauli-invariant unitary ensembles \mathcal{E}_i and \mathcal{E}_o , the shadow channel $\mathcal{M}_{i,o}$ is

$$\mathcal{M}_{i,o}[P_{\vec{a}_i} \otimes P_{\vec{a}_o}] = W_{\mathcal{E}_i}[P_{\vec{a}_i}]W_{\mathcal{E}_o}[P_{\vec{a}_o}]P_{\vec{a}_i} \otimes P_{\vec{a}_o}, \quad (32)$$

where $W_{\mathcal{E}_i}[P_{\vec{a}_i}] = \mathbb{E}_b, \mathbb{E}_{U_i} |\text{Tr}[\hat{\sigma}_i P_{\vec{a}_i}]|^2$ and $W_{\mathcal{E}_o}[P_{\vec{a}_o}] = \mathbb{E}_b, \mathbb{E}_{U_o} |\text{Tr}[\hat{\sigma}_o P_{\vec{a}_o}]|^2$. Hence, for the Pauli-invariant unitary ensemble, $\mathcal{M}_{i,o}^{-1}$ exists iff $W_{\mathcal{E}_i}[\vec{a}_i] > 0, W_{\mathcal{E}_o}[\vec{a}_o] > 0$ for all \vec{a} , and the reconstruction map is defined by

$$\mathcal{M}_{i,o}^{-1}[P_{\vec{a}_i} \otimes P_{\vec{a}_o}] = W_{\mathcal{E}_i}[\vec{a}_i]^{-1}W_{\mathcal{E}_o}[\vec{a}_o]^{-1}P_{\vec{a}_i} \otimes P_{\vec{a}_o}. \quad (33)$$

Now, for the classical shadow tomography for a quantum channel, the sample complexity is upper bounded by the following shadow norm:

$$\|\rho^T \otimes O\|_{\mathcal{E}_T}^2 = \mathbb{E}_{\mathcal{E}_T} \hat{\sigma}[\hat{\sigma}_{i,o}]^2.$$

Next, let us consider the shadow norm in the case where the observable is some Pauli operator and apply this result to the problem of estimating Pauli channels.

Proposition 13. If the observable is taken to be a Pauli operator $P_{\vec{a}}$, then the (squared) shadow norm is equal to

$$\|\rho^T \otimes P_{\vec{a}}\|_{\mathcal{E}_T}^2 = W_{\mathcal{E}_o}[\vec{a}]^{-1} \frac{1}{2^n} \sum_{\vec{a}_i} W_{\mathcal{E}_i}[\vec{a}_i]^{-1} W_{\rho}[\vec{a}_i]. \quad (34)$$

Now, we provide an example of a class of channels for which our results on the classical shadow tomography for quantum channels can be applied.

Example 2. (Estimation of Pauli channels) A quantum channel \mathcal{T} is called a Pauli channel if it can be written as $\mathcal{T}[\cdot] = \sum_{\vec{a} \in \mathbb{V}^n} P_{\vec{a}} P_{\vec{a}}^\dagger [\cdot] P_{\vec{a}}^\dagger$ with $\sum_{\vec{a}} P_{\vec{a}} = 1$. Equivalently, Pauli channels \mathcal{T} can be written as $\mathcal{T}[\cdot] = 1/2^n \sum_{\vec{b}} \lambda_{\vec{b}} \text{Tr}[\cdot P_{\vec{b}}] P_{\vec{b}}$. The task of estimating the coefficients $\{\lambda_{\vec{b}}\}_{\vec{b}}$ of the Pauli channel has been investigated in ref. 49–57. Here, we consider the classical shadow protocol for estimating coefficients $\lambda_{\vec{b}}$ with Pauli-invariant unitary ensembles \mathcal{E}_i and \mathcal{E}_o . The classical shadow is taken to be $\{\mathcal{M}_{i,o}^{-1}[\hat{\sigma}_{i,o}]\}$, and the reconstruction map is given in Proposition 12. To estimate the coefficients $\lambda_{\vec{b}}$, let us consider the observable $P_{\vec{b}} \otimes P_{\vec{b}}$, and take the estimator of the observable to be $\hat{\sigma}_{\vec{b}} = \text{Tr}[\mathcal{M}_{i,o}^{-1}[\hat{\sigma}_{i,o}]P_{\vec{b}} \otimes P_{\vec{b}}]$, where it is easy to verify that $\mathbb{E}[\hat{\sigma}_{\vec{b}}] = \text{Tr}[\mathcal{T}[P_{\vec{b}} \otimes P_{\vec{b}}]] = \lambda_{\vec{b}}$. Then the sample complexity \mathcal{S} needed to accurately predict a collection of 4^n linear target functions $\left\{ \lambda_{\vec{b}} = \text{Tr}[\mathcal{T}[P_{\vec{b}} \otimes P_{\vec{b}}]] \right\}_{\vec{b} \in \mathbb{V}^n}$ with error ϵ and failure probability δ is

$$\mathcal{S} = O\left(\frac{n + \log(1/\delta)}{\epsilon^2} \max_{\vec{b}} W_{\mathcal{E}_o}[\vec{b}]^{-1} W_{\mathcal{E}_i}[\vec{b}]^{-1}\right).$$

DISCUSSION

In this study, we investigated the classical shadow protocol with Pauli-invariant unitary ensembles. First, we provided an explicit formula for the reconstruction map corresponding to the shadow channel and established a connection between the coefficients of the reconstruction map and the entanglement features of the dynamics. Using the shadow norm, we gave explicit sample complexity upper bounds for the estimation task that the classical shadow protocol solves. Finally, we presented two applications of our results. First, we applied our results to locally scrambled unitary ensembles, where we presented explicit formulas for the reconstruction map and the sample complexity bounds. Second, we applied our results to the shadow process tomography of quantum channels with Pauli-invariant unitary ensembles and provided an example where we considered the task of estimating Pauli channels. Our results provide a general framework for classical shadows with a weak assumption on the unitary ensemble in both the noiseless and noisy cases, which can be utilized to predict pertinent properties of quantum states in NISQ devices, including their fidelity, entanglement entropy, and quantum Fisher information.

There are still several interesting unresolved problems: (1) Can one generalize our results to ensembles beyond the Pauli-invariant unitary ensembles? We anticipate that this would be challenging, as a crucial ingredient that we utilize in our proof is that the Pauli ensemble forms a 1-design. This is a very weak assumption, and a more general unitary ensemble may fail to satisfy the 1-design property. That will likely impede a straightforward generalization of our methods. (2) How can one utilize the entanglement feature of the unitary ensemble to improve the performance of the classical shadow across various tasks, such as fidelity estimation?

METHODS

Diagonalization of the shadow channel in the Pauli basis

This section provides a bird's-eye view of the proof of our main result, which centers on the shadow channel $\mathcal{M}(\cdot)$ being diagonal in the Pauli basis. A comprehensive description of our proof is available in Supplementary Note 2. The primary method employed in our proof relies on Fourier analysis with respect to the Pauli basis. The crucial point to establish is as follows:

$$\mathbb{E}_{U, \vec{a}, \vec{b}} \text{Tr}[\hat{\sigma}_{U, \vec{b}} \rightarrow \rho] = \frac{1}{2^{2n}} \sum_{\vec{a} \in \mathcal{V}^n} \mathbb{E}_U \text{Tr}[\hat{\sigma}_{U, \vec{b}} \rightarrow P_{\vec{a}}]^2 \text{Tr}[P_{\vec{a}} \rightarrow \rho] P_{\vec{a}}. \quad (35)$$

This equation is derived using the following two facts: (i) the set of Pauli operators forms an orthonormal basis for the space of n -qubit linear operators, (ii) the Pauli operators obey the following

commutation property: $P_{\vec{a}} \rightarrow P_{\vec{b}} \rightarrow P_{\vec{c}} = (-1)^{\langle \vec{a}, \vec{b} \rangle} P_{\vec{c}}$, where $\langle \cdot, \cdot \rangle$ is the symplectic inner product defined in Supplementary Note 1. The fact that $\mathcal{M}(\cdot)$ is diagonal in the Pauli basis allows us to build the reconstruction map \mathcal{M}^{-1} by simply taking the inverse of the coefficients of $\mathcal{M}(\cdot)$ in the Pauli basis.

DATA AVAILABILITY

Data sharing is not applicable to this article as no datasets were generated or analyzed during the current study.

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AUTHOR CONTRIBUTIONS

K.B., D.E.K., R.J.G. and A.J. designed the study, performed the research, and wrote the manuscript.

COMPETING INTERESTS

The authors declare no competing interests.

ADDITIONAL INFORMATION

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