

# Quantum Codes from Neural Networks

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We report on the usefulness of using neural networks as a variational state ansatz for many-body quantum systems in the context of quantum information-processing tasks. In the neural network state ansatz, the complex amplitude function of a quantum state is computed by a neural network. The resulting multipartite entanglement structure captured by this ansatz has proven rich enough to describe the ground states and unitary dynamics of various physical systems of interest.

In the present paper, we supply further evidence for the usefulness of neural network states to describe multipartite entanglement. We demonstrate that neural network states are capable of efficiently representing quantum codes for quantum information transmission and quantum error correction. In particular, we show that a) neural network states yield quantum codes with a high coherent information for two important quantum channels, the depolarizing channel and the dephrasure channel; b) neural network states can be used to represent absolutely maximally entangled states, a special type of quantum error correction codes. In both cases, the neural network state ansatz provides an efficient and versatile means as variational parametrization of these states.

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# 1. Introduction

The exponential growth of the Hilbert space dimension in the number of particles is both a blessing and curse for quantum science: On the one hand, it is crucial to the widely-believed computational advantage of quantum computers over classical ones, but on the other hand it renders many questions about properties of many-body systems intractable. Yet we know that the “physical” corner of this Hilbert space has to be small: local Hamiltonians with highly-entangled ground states only require a polynomial number of parameters to describe, as do quantum circuits of polynomial depth.

This fact motivates the use of variational representations of quantum states to solve a large class of problems. At the heart of any variational ansatz is the idea to preserve as much information about the quantum state as possible, while discarding irrelevant features. Quantum mechanical properties of a state are fundamentally dictated by its entanglement, which captures quantum correlations between its subsystems.

For instance, correlation length in many-body spin systems is tightly-linked to the existence of a spectral gap [Has07; GH16]. For gapped one-dimensional systems (which follow an entanglement entropy area law), one can use matrix product states (MPS) with polynomial bond dimension to efficiently represent ground states [FNW92; LVV15; Ara+13]; the MPS ansatz has further proven useful e.g. in the study of critical systems [Pir+12] or in the continuum limit [Cue+17]. Other tensor network states include MERA and higher-dimensional variants such as PEPS—applied e.g. in the context of renormalization [Vid07; VC04], and proven similarly successful as part of numerical techniques [Orú14].

A relatively recent development is the use of neural network states as a variational ansatz, where the network is used as a function to calculate the state amplitudes [CT17]. There are many possible neural network architectures to choose from: one proposed model is to use restricted Boltzmann machines (RBMs) to represent e.g. the ground states and unitary dynamics of a transverse-field Ising model and the antiferromagnetic Heisenberg model [CT17], volume-law entanglement and the ground state of even long-range Hamiltonians [DLD17], as well as ground states of various stabilizer Hamiltonians, including the surface code [Jia+18]. While there exist local Hamiltonians that cannot be represented with shallow RBM architectures, it has been shown that deep feed-forward (FF) networks can in fact represent *any* physical state [GD17].

Apart from describing the physics of many-body systems, entanglement also plays a crucial role in information-processing tasks: teleportation [Ben+93], superdense coding [BW92], and entanglement-assisted classical [Ben+99] and quantum [DHW04] communication all build on *bipartite* entanglement as a resource. In contrast, for certain tasks

such as quantum information transmission through many uses of a quantum channel, or the encoding of quantum information in quantum error-correction codes, the crucial property is *multipartite entanglement*, which encapsulates correlations among all the constituents of the system simultaneously [Has07].

## 1.1. Main Results of this Paper

We demonstrate that neural network states with only polynomially many parameters in the system size (which, in this context, we call *efficient*) are capable of representing quantum codes for quantum information transmission and quantum error correction. In particular, we show on the one hand that neural network states can efficiently represent quantum codes with a high coherent information (CI) for two important quantum channels, the depolarizing channel and the dephrasure channel [LLS18a]. On the other hand, we show that neural network states can be used to parametrize so-called “absolutely maximally entangled” (AME) states. These AME states, defined on  $n$  systems of local dimension  $d$  each, are examples of quantum error correction codes with the property that they are completely mixed after tracing out at least half of the systems. Besides their quantum error correction capabilities, AME states are useful in multi-user information-theoretic tasks such as open-destination teleportation, secret sharing or entanglement swapping that require maximal entanglement across different choices of bipartitions [HC13; Hel+12]. The properties of both quantum codes with high coherent information and AME states are the result of the non-trivial multipartite entanglement present in these states.

*The main result of this paper is that for both high-CI states and AME states, a neural network state ansatz is able to faithfully represent this multipartite entanglement, which we demonstrate empirically for small problem instances. We provide numerical evidence that the variational ansatz vastly outperforms a full state parametrization for the respective learning tasks, and that FF networks converge faster than RBMs with comparable parameter counts. For the depolarizing channel, we further constructively prove that a series of high-CI states (repetition codes, and products thereof) can be obtained efficiently with both an RBM and a FF architecture.*

## 1.2. Structure of this Paper

In the following sections, we present our main results about representing quantum codes with neural network states. First, we show in Sec. 2 how tensor products of repetition codes—i.e. the known optimal codes for  $k \leq 9$  uses of a depolarizing channel—can be efficiently represented using FF and RBM networks, and comment on the trainability

of our chosen network architectures. Second, for the dephrasure channel [LLS18a] we show in Sec. 3 how the neural network state ansatz yields even better codes than can be found using “traditional” numerical methods. Third, in Sec. 4 we demonstrate how known examples of AME states can be efficiently represented using neural networks, and we comment on the trainability of the network architectures that we used. We conclude in Sec. 5.

In the appendices, we give more details about certain aspects of the paper. In App. A we discuss the quantum capacity of a quantum channel in more detail and explain some terminology. In App. B, we give the product repetition codes yielding the highest rate for a fixed number  $n$  of channel uses of the qubit depolarizing channel. In App. C we recapitulate some of the main facts about the dephrasure channel that are derived by one of the authors and collaborators in [LLS18a]. In App. D we provide some background information on absolutely maximally entangled states, and prove a useful bound on a trace distance parameter indicating how close a state is to being absolutely maximally entangled. In App. E we review neural network states and some common neural network architectures used to define them. We also discuss possible encodings of  $d$ -ary input strings to neural networks, and comment on the role of activation functions for quantum codes; furthermore, we propose a novel NN Schmidt decomposition ansatz, which we benchmark against a full NN parametrization for the depolarizing channel. In App. F we give the analytical proof how tensor products of the known optimal codes for  $k \leq 9$  can be efficiently represented using neural networks, comment on a variant of RBMs (called deep Boltzmann machines), and the Schmidt ansatz. In App. G we give a high-level explanation of the global derivative-free numerical optimization techniques used in our paper. Finally, we provide additional numerical data for our results in App. H.

We encourage researchers to adopt our methods by providing full access to our code (in C++ and MATLAB) that was used to obtain the numerical results of this paper. These code files can be found in the “Ancillary files” section of the arXiv post of this paper [Anc]. In MATLAB, we made use of the MATLAB Global Optimization Toolbox, as well as quantinf [Cub05] and QETLAB [Joh16]. In C++, we made use of NLOpt [Joh] with the CCSA algorithm [Sva02] as well as PAGMO [BIM18].

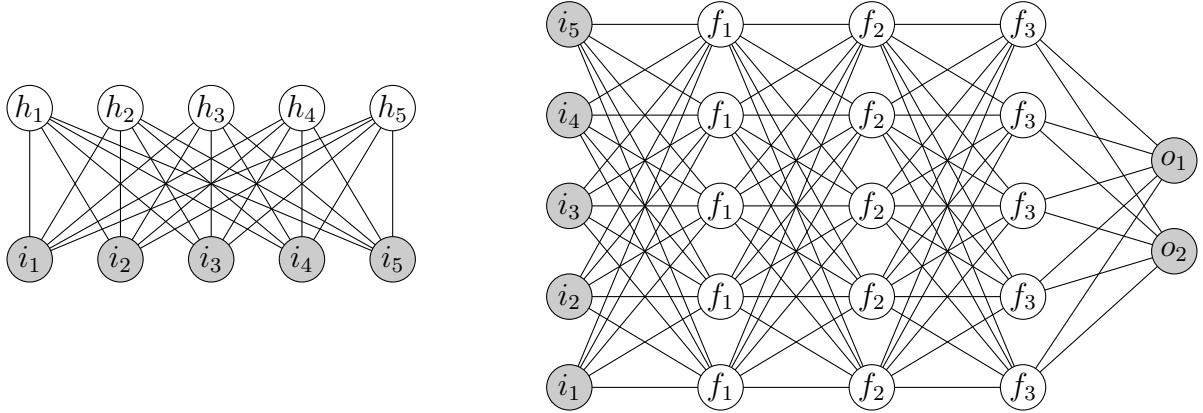


Figure 1: Left: Restricted Boltzmann machine (RBM) with five input layers, and five hidden nodes. Right: Feed forward neural network with five input nodes, one output node, and three fully-connected hidden layers of size five each. Each line represents one real value being propagated forward from node to node; the  $f_i$  are non-linear activation functions (e.g. sigmoid, ReLU, cos, see Sec. E.6 for a discussion) applied to an affine transformation of the node inputs (see Eq. 38).

## 2. Representing the Best Known Codes for the Depolarizing Channel

The *depolarizing channel* is used as a model to describe qubit decoherence in a noisy environment. For a qubit in a state described by the density operator  $\rho$ , and for a real parameter  $p \in [0, 4/3]$ , the action of the channel is given by

$$\mathcal{D}_p(\rho) := (1 - p)\rho + p \text{tr}(\rho)(|0\rangle\langle 0| + |1\rangle\langle 1|)/2, \quad (1)$$

i.e. the original state  $\rho$  is replaced by the maximally mixed state with ‘probability’  $p$  (for  $p \leq 1$ ); in other words, if on the Bloch sphere  $\rho$  has spin polarization vector  $\vec{x}$ , the channel  $\mathcal{D}_p$  shrinks  $\vec{x}$  by a factor  $1 - p$ .

The maximum possible rate at which quantum information can be transmitted faithfully through a channel  $\mathcal{N}$  is given by the *quantum capacity*  $Q(\mathcal{N})$ , which can be expressed as [Llo97; Sho02; Dev05]

$$Q(\mathcal{N}) = \lim_{n \rightarrow \infty} \frac{1}{n} Q^{(1)}(\mathcal{N}^{\otimes n}) = \sup_{n \in \mathbb{N}} \frac{1}{n} Q^{(1)}(\mathcal{N}^{\otimes n}). \quad (2)$$

Here, the *channel coherent information*  $Q^{(1)}(\mathcal{N})$  is defined as

$$Q^{(1)}(\mathcal{N}) = \max_{|\psi\rangle_{RA}} Q^{(1)}(\psi_{RA}, \mathcal{N}) = \max_{\psi_{RA}} S(\mathcal{N}(\psi_A)) - S((\text{id}_R \otimes \mathcal{N})(\psi_{RA})), \quad (3)$$

with the von Neumann entropy  $S(\rho) := -\text{tr}(\rho \log(\rho))$ . We refer to (Sec. A) for a more detailed definition and discussion of the quantum capacity.

Eq. 2 for the quantum capacity involves the evaluation of the channel coherent information  $Q^{(1)}(\cdot)$  over an unbounded number of channel uses, and renders the quantum capacity  $Q(\mathcal{N})$  intractable to compute in general (Sec. A). This is because the coherent information can be strictly superadditive for some channels such as the depolarizing channel [DSS98]: there exist codes e.g. for  $p \approx 0.2531$  such that  $Q^{(1)}(\mathcal{D}_p^{\otimes 5}) > 5Q^{(1)}(\mathcal{D}_p)$  (in fact, for this  $p$ , we have  $Q^{(1)}(\mathcal{D}_p) = 0$ ). Operationally, positive channel coherent information guarantees—by the quantum capacity theorem Eq. 2—the existence of entanglement-generating protocols with a positive rate even in the high-noise regime [Llo97; Sho02; Dev05]; the challenge is thus to find quantum codes  $\chi_n$  for  $n$  channel copies which maximize  $Q^{(1)}(\chi_n, \mathcal{N}^{\otimes n})$ . More generally, we consider the task of finding quantum codes for which  $Q^{(1)}(\chi_n, \mathcal{N}^{\otimes n}) > 0$ , especially in the situation where  $Q^{(1)}(\mathcal{N}) = 0$ .

For the depolarizing channel, the single-letter channel coherent information  $Q^{(1)}(\mathcal{D}_p)$  is maximized by a Bell state  $\frac{1}{\sqrt{2}}(|0\rangle_R|0\rangle_A + |1\rangle_R|1\rangle_A)$ , and evaluates to

$$Q^{(1)}(\mathcal{D}_p) = 1 + \left(1 - \frac{3p}{4}\right) \log \left(1 - \frac{3p}{4}\right) + \frac{3p}{4} \log \frac{p}{4}. \quad (4)$$

$Q^{(1)}(\mathcal{D}_p)$  remains positive up to the threshold at  $p = 0.25238$  (the *threshold* is defined as the highest  $p$  for which  $Q^{(1)}(\mathcal{D}_p) \geq 0$ ). The next highest thresholds are achieved for  $n = 3$  and 5 channel copies and an  $n$ -repetition code

$$|\phi_n\rangle = \frac{1}{\sqrt{2}}(|0\rangle_R|0\rangle_A^{\otimes n} + |1\rangle_R|1\rangle_A^{\otimes n}), \quad (5)$$

for which the channel coherent information  $Q^{(1)}(\phi_n, \mathcal{D}_p^{\otimes n})$  reaches zero at  $p = 0.25350$  and  $p = 0.25380$ , respectively. Both in terms of the rate and the threshold, these repetition codes are the best known codes up to 9 channel copies, which is discussed in more detail in (Sec. B).

We show in the following that a variational neural network ansatz achieves these codes for the depolarizing channel, and contrast the various architectures on an empirical level. With respect to a fixed basis  $\{|i\rangle\}_{i=0}^{d-1}$ , a general quantum state on  $n$  qudits of dimension  $d$  can be written as

$$|\psi_{n,d}\rangle = \frac{1}{C} \sum_{i^n \in [d]_0^n} \psi(i^n) |i^n\rangle \in (\mathbb{C}^d)^{\otimes n}, \quad (6)$$

where  $C$  is a normalization constant, and we write  $[d]_0 := \{0, \dots, d-1\}$ . For the depolarizing channel,  $|\psi_{n,d}\rangle$  is a joint state on the reference and input qubits of local dimension  $d = 2$ .

As a variational amplitude function  $\psi(i^n)$  we use both an RBM architecture as well as an FF architecture with a cos activation function in the first hidden layer, and ReLU

in all subsequent hidden layers, a setup which has been shown to perform well in the context of representing quantum states of local Hamiltonians [CL18], and which we found to outperform an only-ReLU-layer architecture as well. Furthermore, we propose a Schmidt-ansatz similar to Eq. 6 given for  $2l$  qubits by

$$|\psi_{2l}\rangle = \frac{1}{C} \sum_{i^l \in [d]_0^l} \psi(i^l) |i^l\rangle_R |i^l\rangle_A. \quad (7)$$

This approach reduces the number of degrees of freedom required to parametrize  $|\psi_{2l}\rangle$ , but enforces the environment  $R$  to have the same dimension as the system  $A$ , introducing redundancy e.g. for a repetition code which ordinarily only requires a single purifying qubit. It furthermore introduces a choice of basis for the channel input qubits, rendering this ansatz less general than the one in Eq. 6.

Using an explicit construction, we show that both FF and RBM architectures can efficiently represent products of repetition codes (Sec. F): given  $k$  repetition codes on  $n_1, \dots, n_k$  qubits, respectively, an RBM with  $\prod_i n_i$  visible units and  $k$  hidden nodes can represent the corresponding state amplitudes, and a FF net with first cos and second ReLU hidden layer width  $k$ , and a single final ReLU node suffices.

Empirically, we contrast FF, RBM and their corresponding Schmidt variants as a variational ansatz  $\psi_n$  to maximize  $Q^{(1)}(\psi_n, \mathcal{D}_p^{\otimes n})$ ; in comparison with a full state vector on  $n$  qubits with  $2 \times 2^n$  real parameters, we can see a significant improvement in convergence speed (see Fig. 2), both in the case that the best-known code is a single repetition code for three channel uses, or a three times one product repetition code (see (Sec. B) for an explanation of this terminology). For both FF and RBM architectures, the Schmidt ansatz Eq. 7 surpasses the standard parametrization Eq. 6, which is likely due to the significantly-reduced parameter count. FF networks further outperform RBM architectures with comparable parameter counts on three and four channel uses of a depolarizing channel, which we verified with various global derivative-free optimization techniques (Sec. G) to reduce the likelihood of a systematic bias in our numerical findings (Sec. H).

### 3. New Codes for the Dephrasure Channel

The neural network ansatz proves particularly useful in finding good quantum codes for the *dephrasure channel* that was introduced recently in [LLS18a]. It is defined in terms of probabilities  $p, q \in [0, 1]$  as

$$\mathcal{N}_{p,q}(\rho) = (1 - q)((1 - p)\rho + pZ\rho Z) + q \text{tr}(\rho)|e\rangle\langle e|, \quad (8)$$

where  $Z = |0\rangle\langle 0| - |1\rangle\langle 1|$  is the Pauli  $Z$ -operator, and  $|e\rangle$  is an erasure flag that is orthogonal to the input space. The name ‘dephrasure’ is derived from the fact that  $\mathcal{N}_{p,q}$  first dephases an input state in the  $Z$ -basis with probability  $p$ , and then erases it with probability  $q$ . Despite the fact that both dephasing and erasure noise are well-understood in terms of quantum information transmission, the dephrasure channel—a concatenation of the two—exhibits superadditivity of coherent information for as little as two uses of the channel [LLS18a]. Via the neural network state ansatz, we find new quantum codes which further increase the superadditivity threshold of coherent information for the dephrasure channel.

In the following, we focus our attention to the  $(p, 3p)$ -diagonal in the  $(p, q)$ -plane, and investigate  $k = 3, 4$  uses of the dephrasure channel  $\mathcal{N}_{p,3p}$  for the values  $p = 0.115, 0.116, 0.117$ . In this high-noise regime the single-letter coherent information is not optimal, and there exist various codes—such as repetition codes and more general  $Z$ -diagonal codes—that show superadditivity of the coherent information, i.e.,  $Q^{(1)}(\mathcal{N}_{p,3p}^{\otimes n}) > nQ^{(1)}(\mathcal{N}_{p,3p})$  for  $n \geq 2$  (Sec. C).

To obtain new codes, we used a feed-forward network as described in Fig. 1 with four hidden layers of width  $2k$  each, cos as the activation function in the first layer, and ReLU as the activation function in the remaining layers. The neural network parameters were optimized using the particle swarm optimization algorithm followed by pattern search (Sec. G). The resulting codes  $\nu_3$  on  $k = 3$  input qubits and  $\nu_4^{(1)}$  and  $\nu_4^{(2)}$  on  $k = 4$  input qubits achieve higher coherent information rates than the best known codes obtained in [LLS18a]; for a comparison see Tab. 1.

Since the dephrasure channel is defined in terms of a  $Z$ -dephasing (see eq. 8), we would expect optimal codes to be diagonal in the computational basis (the eigenbasis of  $Z$ ). Here, we call a pure code state  $|\phi\rangle_{RA^k}$  *diagonal* with respect to a certain basis, if the channel input state  $\phi_{A^k} = \text{tr}_R \phi_{RA^k}$  is diagonal with respect to that basis (and hence invariant under dephasing). However, the codes  $\nu_3$  and  $\nu_4^{(2)}$  have *off-diagonal elements* with respect to the computational basis (Sec. C). These new codes therefore challenge the conjectured optimality of diagonal codes, adding further evidence that the dephrasure channel exhibits exotic behavior despite its simple form.

## 4. Representing Absolutely Maximally Entangled States

Absolutely maximally entangled (AME) states are  $n$ -partite states having maximal correlation across any bipartition of the  $n$  parties into equal halves. These states are certain examples of quantum error correction codes, whose intricate multipartite

$p$	$k$	code	rate	NN code	rate
0.115	3	$\chi_3$	$1.0191 \times 10^{-3}$	$\nu_3$	$1.0201 \times 10^{-3}$
0.116	4	$\theta_4$	$4.6615 \times 10^{-4}$	$\nu_4^{(1)}$	$4.6638 \times 10^{-4}$
0.117	4	$\theta_4$	$1.3797 \times 10^{-4}$	$\nu_4^{(2)}$	$1.6401 \times 10^{-4}$

Table 1: Comparison of the rates of dephrasure codes for  $k = 3, 4$  channel uses of the dephrasure channel  $\mathcal{N}_{p,3p}$  with  $p \in \{0.115, 0.116, 0.117\}$ . While  $\chi_3$  and  $\theta_4$  are codes that were found using ‘traditional’ numerical methods, the codes  $\nu_3$ ,  $\nu_4^{(1)}$  and  $\nu_4^{(2)}$  were found using the neural network ansatz (see (Sec. C) for a definition of these codes).

entanglement structure mediates correlations between different subsets of the constituent systems.

AME states can be used as a resource for multi-user information-theoretic tasks such as open-destination teleportation, secret sharing or entanglement swapping that require maximal entanglement across different choices of bipartitions [HC13; Hel+12]. In a holographic context, where AME states are referred to as *perfect tensors*, they provide examples of holographic error correction codes [LS15; Pas+15; Li+17]. More generally, an arbitrary AME state on  $n$  qudits can be interpreted as a quantum error correction code of distance  $\lfloor \frac{n}{2} \rfloor + 1$  encoding 1 logical qudit of dimension  $d$  in  $n$  physical qudits [Sco04].

To define absolutely maximally entangled (AME) states in a precise way, we consider a pure state  $|\psi_{n,d}\rangle \in (\mathbb{C}^d)^{\otimes n}$  on  $n$  qudits of local dimension  $d$ . For a subset  $\mathcal{S} \subset [n] := \{1, \dots, n\}$  of the  $n$  qudits we denote by  $\rho_{\mathcal{S}} = \text{tr}_{\mathcal{S}^c} \psi_{n,d}$  the marginal of  $\psi_{n,d}$  on  $\mathcal{S}$ . Then  $\psi_{n,d}$  is AME if  $\rho_{\mathcal{S}} = \frac{1}{|\mathcal{S}|} I_{\mathcal{S}}$  for every  $\mathcal{S} \subset [n]$  with  $|\mathcal{S}| = \lfloor \frac{n}{2} \rfloor$ . We use the notation  $\text{AME}(n, d)$  for an AME state on  $n$  qudits of local dimension  $d$ .

Since an AME state is maximally entangled across all possible bipartitions into equal halves, monogamy of entanglement puts an obstruction on their existence [CKW00]. Furthermore, the fact that AME states are particular quantum error correction codes yields additional constraints via weight enumerator theory [SL97; Rai98]. Consequently, AME states do not exist for all  $(n, d)$  (Sec. D). For example, it is known that there is no  $\text{AME}(4, 2)$  state [HS00]. On the other hand, an example of an  $\text{AME}(4, 3)$  state is  $|\Omega_{4,3}\rangle = \frac{1}{3} \sum_{i,j=0,1,2} |i\rangle |j\rangle |i+j(3)\rangle |i+2j(3)\rangle$ , where  $k(d) \equiv k \pmod{d}$ .

The property of  $\psi_{n,d}$  being absolutely maximally entangled is related to the *linear entropy*  $S_L(\rho_S) = \frac{d^m}{d^m - 1}(1 - \text{tr}(\rho_S^2))$  of the marginals  $\rho_S$  for  $\mathcal{S} \subset [n]$  with  $|\mathcal{S}| = \lfloor \frac{n}{2} \rfloor$ . Defining for  $m = 1, \dots, \lfloor \frac{n}{2} \rfloor$  the average linear entropy

$$Q_m(\psi_{n,d}) := \binom{n}{m}^{-1} \sum_{\mathcal{S} \subset [n]: |\mathcal{S}|=m} S_L(\rho_S), \quad (9)$$

a pure state  $\psi_{n,d}$  is AME if and only if  $Q_{\lfloor \frac{n}{2} \rfloor}(\psi_{n,d}) = 1$  [Sco04]. Hence, to search for AME( $n, d$ )-states  $\psi_{n,d}$ , we can use Eq. 9 with  $m = \lfloor \frac{n}{2} \rfloor$  as the objective function and optimize the parameters in the ansatz for  $\psi_{n,d}$  such that  $Q_{\lfloor \frac{n}{2} \rfloor}(\psi_{n,d}) \approx 1$ . As before, we use a neural network state ansatz for  $\psi_{n,d}$ .

We demonstrate in Fig. 3 that parametrizing  $\psi_{n,d}$  with a neural network state ansatz yields AME( $n, d$ )-states for the pairs  $(n, d) = (3, 6)$ ,  $(4, 4)$ , and  $(4, 7)$ . For the numerical optimization, we use the artificial bee colonization algorithm, followed by pattern search and a final round of gradient search. These choices of parameters are only exemplary, and the neural network state ansatz is capable of representing AME( $n, d$ )-states also for other pairs  $(n, d)$ , e.g.,  $(3, 3)$ ,  $(4, 3)$ , and  $(4, 5)$ . In the last three cases, the convergence is remarkably fast and only takes a few iterations of optimization algorithms such as ABC or PSO to reach a value of  $Q_{\lfloor \frac{n}{2} \rfloor}$  sufficiently close to 1.

To assess our numerical results, we introduce an ‘average trace distance’ parameter

$$D_m(\psi_{n,d}) := \binom{n}{m}^{-1} \sum_{\mathcal{S} \subset [n]: |\mathcal{S}|=m} \|\rho_S - \pi_S\|_1, \quad (10)$$

where  $\pi_S := \frac{1}{|\mathcal{S}|} I_{\mathcal{S}}$  denotes the completely mixed state, and  $\|X\|_1 = \text{tr} \sqrt{X^\dagger X}$  is the trace norm of an operator  $X$ . The parameter  $D_m(\psi_{n,d})$  measures the average trace distance of the marginals of a state  $\psi_{n,d}$  on  $m$  subsystems to the completely mixed state. Clearly,  $D_{\lfloor \frac{n}{2} \rfloor}(\psi_{n,d}) = 0$  if and only if  $\psi_{n,d}$  is AME. We prove in (Sec. D) that

$$D_m(\psi_{n,d}) \leq \sqrt{2 \log[d^m - (d^m - 1)Q_m(\psi_{n,d})]}. \quad (11)$$

This bound allows us to relate a value of  $Q_m$  to how close (on average) in trace distance a state is to being AME (see Fig. 3).

## 5. Discussion

In this work, we have shown that quantum codes for noisy quantum communication and certain quantum error correction codes can be modeled with various neural network representations. In particular, we investigated quantum codes that yield high coherent information for the quantum depolarizing channel and a novel channel called the

$n$	$d$	architecture	encoding	hidden layer
3	6	FF	binary	(12, 12, 12)
		RBM	binary	12
4	4	FF	binary	(8, 8, 8)
		RBM	binary	8
4	7	FF	scaled	(4, 4, 4)
		RBM	scaled	4

Table 2: Encodings and network architectures used to represent AME( $n, d$ )-states as plotted in Fig. 3. For the FF nets, the hidden layers are denoted by  $(M_i)_i$ , where  $M_i$  is the width of the  $i$ -th hidden layer. We always use cos in the first hidden layer and ReLU in the following hidden layers. For the RBM net, we list the width of the single hidden layer. The encodings are defined in (Tab. 4).

dephrasure channel [LLS18a]. For  $k \leq 6$  of the depolarizing channel, we analyzed the representative power of neural network states with regards to the best known codes, repetition codes, and benchmarked how well they can be trained using a variety of global optimization algorithms. For  $k \leq 4$  uses of the dephrasure channel, we showed how the neural network ansatz can be used to find codes that surpass the best known codes found with traditional numerical methods. Finally, we demonstrated how neural network states can represent absolutely maximally entangled states on  $n$  qudits of local dimension  $d$  for an array of pairs  $(n, d)$ .

An interesting question is, of course, whether a neural network state ansatz can be used to find better quantum codes for the depolarizing channel in the high noise regime: either in terms of a higher rate than, say, the 5-repetition code right below the noise threshold, or in terms of increasing the noise threshold itself. Our results indicate that in order to find such codes outperforming the repetition codes (or products thereof), one ought to increase the number of channel copies beyond 5, resulting in code states on 10 or more input qubits. While the (polynomial) scaling of the neural network ansatz in the number of input qubits is favorable, the calculation of the coherent information is the bottleneck here: The computation for a code on  $k$  qubits requires diagonalizing a dense  $4^k \times 4^k$  matrix, which scales exponentially in runtime with the number of qubits. Due to these computational limitations, evaluating the coherent information for  $k \gtrsim 7$  channel uses is thus an infeasible undertaking, and we would need to find an alternative approach—e.g. by exploiting symmetry considerations, or an approximate cost function that is faster to compute (see e.g. [WBS14], with the added difficulty that the coherent information is the difference between two entropies).

Furthermore, it could be possible that better quantum codes lie in maxima of measure almost zero, while the repetition code maxima dominate the potential landscape, making it difficult to find codes that surpass repetition codes. In fact, in all our simulations for  $k \leq 6$  channel uses, the variational NN ansatz converges to product repetition codes. Our results might be seen as indication that, among the states that can be represented using a neural network, repetition codes are in fact optimal for  $k \leq 6$  copies of the depolarizing channel. We note that our techniques of finding quantum codes using neural network states can also be applied to other channels such as generalized Pauli channels, which includes the depolarizing channel. A thorough investigation of other channels in this class, such as the BB84 channel [BB84], is the subject of ongoing work.

We also applied our ansatz to search for AME( $n, d$ )-states for values of  $(n, d)$  for which it is unknown yet whether these states exist. The smallest-dimensional instances of these cases are  $(4, 6)$  and  $(7, 4)$  (Sec. D). For  $(n, d) = (4, 6)$  the best value we obtained was  $Q_2(\psi_{4,6}) \approx 0.9956$ , which translates via Eq. 11 to a bound on the average trace distance parameter of  $D_2(\psi_{4,6}) \lesssim 0.6429$ . The state  $\psi_{n,d}$  achieving these values is an RBM state with binary encoding and a hidden layer width of  $M = 12$ . For  $(n, d) = (7, 4)$ , we obtained  $Q_3(\psi_{7,4}) \approx 0.9962$ , corresponding to  $D_3(\psi_{7,4}) \lesssim 0.7870$ , achieved by an FF state with binary encoding and hidden layers  $(14, 14, 14)$  with activation functions  $(\cos, \text{ReLU}, \text{ReLU})$ . These results suggest that, assuming AME states do exist in these cases, one has to tweak the neural network ansatz or the numerical methods, or both, in order to obtain numerical instances of AME states.

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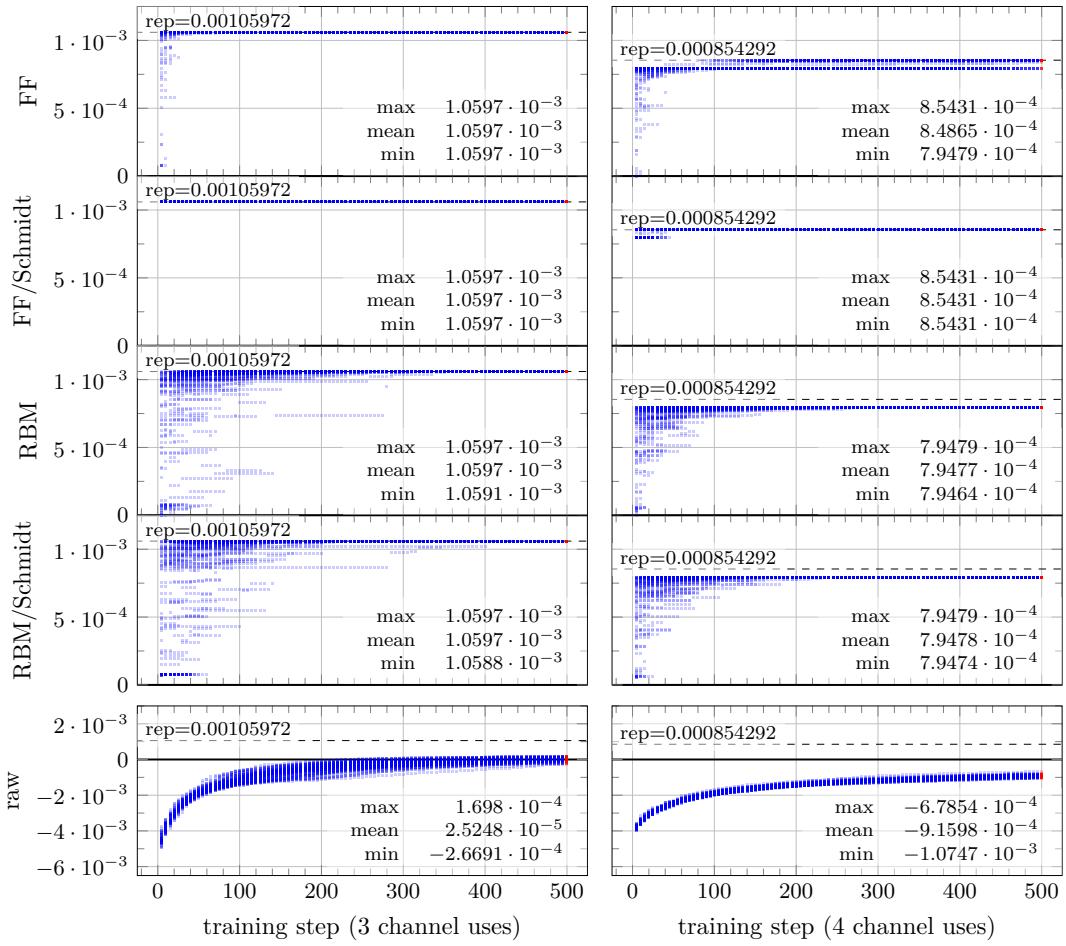


Figure 2: Training convergence of a particle swarm algorithm maximizing the CI of three resp. four copies of the depolarizing channel  $\mathcal{D}_p$ , with noise parameter  $p = 0.2523$ . Plotted are the best candidates of 80 threads à 100 particles for every training step from 0 to 1000. The final candidate distribution, and the outcome of other optimization algorithms can be seen in (Sec. H); For three channel uses, a three-repetition code maximizes the coherent information, whereas for four channel uses, a product code of a three-repetition and single-repetition code is optimal. Plotted are FF (feed-forward net, 140 resp. 234 real parameters), FF/Schmidt (Schmidt representation obtained from a feed-forward net, 40 resp. 65 real parameters), RBM (restricted Boltzmann machine with hidden layer width 9, 138 resp. 232 real parameters), RBM/Schmidt (Schmidt representation obtained from an RBM with hidden layer width 9, 39 resp. 64 real parameters), and raw (parametrizing the full state vector, 128 resp. 512 real parameters); note that the FF and RBM representations are in fact overspecified for three channel uses.

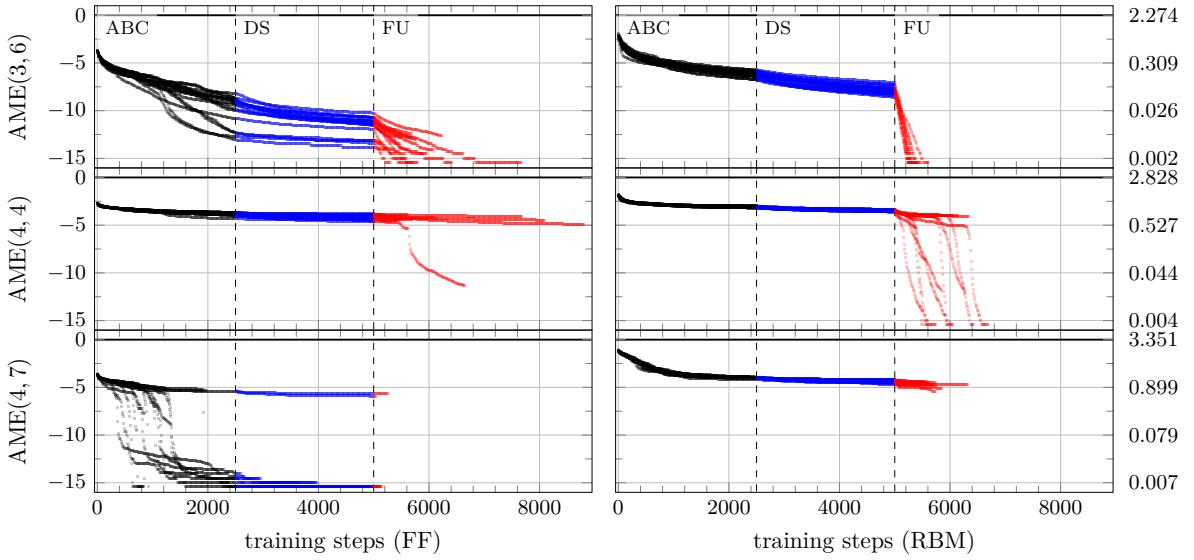


Figure 3: Training convergence for representing  $\text{AME}(n, d)$ -states for  $(n, d) \in \{(3, 6), (4, 4), (4, 7)\}$  using consecutive steps of artificial bee colonization (ABC), direct search (DS), and gradient search (FU). On the left y-axis we plot the quantity  $\ln(1 - Q_m)$ , and on the right y-axis we plot the bound Eq. 11 on the average trace distance parameter  $D_m$  defined in Eq. 10. The encodings used to represent the  $d$ -ary input strings, as well as the network architectures for the FF and RBM nets are listed in Tab. 2.

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## A. The Quantum Capacity of a Quantum Channel

A point-to-point communication link between quantum systems can be modeled by a *quantum channel*. For quantum systems  $A$  and  $B$  with underlying Hilbert spaces  $\mathcal{H}_A$  and  $\mathcal{H}_B$ , respectively, a quantum channel  $\mathcal{N}: A \rightarrow B$  is a linear, completely positive, trace-preserving map between the algebras of linear operators  $\mathcal{B}(\mathcal{H}_A)$  and  $\mathcal{B}(\mathcal{H}_B)$ .

The communication capabilities of a quantum channel are characterized by various *capacities*, depending on what kind of information one attempts to transmit faithfully through the channel. The *quantum capacity*  $Q(\mathcal{N})$  of a quantum channel  $\mathcal{N}: A \rightarrow B$  characterizes the optimal rate of faithful quantum information transmission through the channel.  $Q(\mathcal{N})$  can be defined in terms of the operational task of *entanglement generation* as follows.

Suppose Alice, the sender, prepares a pure state  $\psi_{RA^n}$  in her laboratory and sends the  $A^n$ -part to Bob through  $n$  independent uses of the quantum channel  $\mathcal{N}$ .<sup>1</sup> Upon receiving the quantum systems from Alice, Bob applies some decoding operation  $\mathcal{D}_n: B^n \rightarrow R'$  to the output, yielding the final state  $\sigma_{RR'} = (\text{id}_R \otimes \mathcal{D}_n \circ \mathcal{N}^{\otimes n})(\psi_{RA^n})$ . The goal for Alice and Bob is to obtain a final state  $\sigma_{RR'}$  that is close (in a suitable distance measure) to a maximally entangled state  $|\Phi^{M_n}\rangle_{RR'}$  of Schmidt rank  $M_n$ , i.e.,  $|\Phi^{M_n}\rangle_{RR'} = M_n^{-1/2} \sum_{i=1}^{M_n} |i\rangle_R \otimes |i\rangle_{R'}$  for some basis  $\{|i\rangle\}_i$ . If there is an entanglement generation protocol such that  $\sigma_{RR'}$  converges to  $|\Phi^{M_n}\rangle_{RR'}$  with respect to the chosen distance as  $n \rightarrow \infty$ , then  $\lim_{n \rightarrow \infty} \frac{1}{n} \log M_n$  is called an *achievable rate*. The quantum capacity  $Q(\mathcal{N})$  is defined as the supremum over all achievable rates.

The formula 2 for the quantum capacity stated in the main text involves the evaluation of the channel coherent information  $Q^{(1)}(\cdot)$  over an (in principle) unbounded number of channel copies. If the channel coherent information is *weakly additive*,  $Q^{(1)}(\mathcal{N}^{\otimes n}) \leq nQ^{(1)}(\mathcal{N})$ , then the regularization in Eq. 2 is not necessary, and  $Q(\mathcal{N}) = Q^{(1)}(\mathcal{N})$ . Weak additivity of the channel coherent information is only known to hold for certain classes of channels such as degradable channels [DS05]. Moreover, there are known examples of quantum channels for which the channel coherent information is strictly *superadditive*,  $Q^{(1)}(\mathcal{N}^{\otimes n}) > nQ^{(1)}(\mathcal{N})$  for some  $n$ , rendering the regularization over  $n$  in the quantum capacity formula 2 necessary in general [DSS98]. However, for so-called *low-noise* channels that are close in diamond norm to a noiseless channel, the effect of superadditivity of coherent information cannot be too large, and the single-letter coherent information is essentially the right answer [LLS18b; Sut+17].

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<sup>1</sup>That is, Alice uses the  $A^n$ -part of  $\psi_{RA^n}$  as the input to the channel  $\mathcal{N}^{\otimes n}$ .

## A.1. Achievability of Channel Coherent Information and Quantum Codes

An important part of the quantum capacity theorem in Eq. 2 is the fact that the channel coherent information is an *achievable rate* [Llo97; Sho02; Dev05]:

$$Q(\mathcal{N}) \geq Q^{(1)}(\mathcal{N}). \quad (12)$$

Using block codes, this can be generalized to  $Q(\mathcal{N}) \geq \frac{1}{n}Q^{(1)}(\mathcal{N}^{\otimes n})$  for all  $n \in \mathbb{N}$ . The rough proof idea of Eq. 12 is the following: Assume that  $|\psi\rangle_{RA}$  is a pure state with strictly positive coherent information,  $Q^{(1)}(\psi, \mathcal{N}) > 0$ . Once Alice and Bob share  $k$  copies of the state  $\sigma_{RB} = (\text{id}_R \otimes \mathcal{N})(\psi_{RA})$  (which they can achieve by Alice sending the  $A^k$  part of the state  $\psi_{RA}^{\otimes k}$  to Bob through  $\mathcal{N}^{\otimes k}$ ) for a sufficiently large  $k$ , there is a protocol defined in terms of the typical subspaces of  $\sigma_{RB}^{\otimes k}$  that allows Alice and Bob to generate entanglement between them at a rate of  $r - \delta$  for arbitrarily small  $\delta \in (0, r)$ , where  $r$  is equal to the coherent information of the state  $\sigma$ , that is,  $r = I(R\rangle B)_\sigma = Q^{(1)}(\psi, \mathcal{N})$ .

In this operational picture, we can think of  $\psi_{RA}$  as the *inner code*, whereas the protocol manipulating  $\sigma_{RB}^{\otimes k}$  is the *outer code*. The rate at which the full protocol generates entanglement is solely determined by the (strictly positive) coherent information of the inner code  $\psi_{RA}$ . In this paper, we refer to the inner code  $\psi_{RA}$  simply as a *quantum code*.

## B. Product Repetition Codes for the Depolarizing Channel

In this appendix, we discuss the known optimal codes for the depolarizing channel. For  $p \lesssim 0.2519$ , the single-letter coherent information Eq. 4 is optimal. For  $0.2519 \lesssim p \lesssim 0.2533$ , the 3-repetition code  $\phi_3$  (defined in Eq. 5) is optimal, while for  $0.2533 \lesssim p \lesssim 0.2538$  the 5-repetition code  $\phi_5$  is optimal. The point  $p \simeq 0.2538$  marks the highest threshold for a single repetition code. This threshold can be further extended using the concatenated codes of [SS07; FW08].<sup>2</sup> We summarize this in Fig. 4, where we compare the repetition codes and their rates and thresholds.

The above codes are the best known *information-theoretic* codes, yielding the best lower bounds on the quantum capacity of the depolarizing channel by Eq. 12. However,

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<sup>2</sup> Note that these concatenated codes require at least 10 channel uses of the depolarizing channel, and thus their rate is far lower than the rates of the codes just described. Furthermore, investigating  $n \geq 10$  channel uses of the depolarizing channel is at the moment out of reach for our numerical methods. For these reasons, we focus on the regime  $p \leq 0.2538$  within the threshold of  $\phi_5$ .

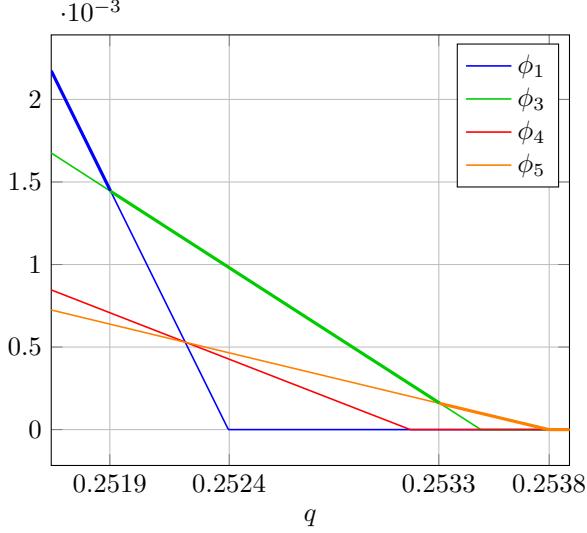


Figure 4: Rates and thresholds for the coherent information of repetition codes  $\phi_n$  for the depolarizing channel  $\mathcal{D}_p^{\otimes n}$  with  $p \in [0.2516, 0.2539]$  and  $n = 1, 3, 4, 5$ . The enveloping thick line marks the known optimal coherent information for the depolarizing channel (up to the concatenated codes of [SS07; FW08], which are not shown here).

in numerical investigations we are facing a slightly different problem of maximizing the  $n$ -coherent information  $\frac{1}{n}Q^{(1)}(\psi_n, \mathcal{D}_p^{\otimes n})$  over quantum codes  $\psi_n$  for *fixed*  $n$ , that is, solving

$$\operatorname{argmax}_{\psi_n} \frac{1}{n}Q^{(1)}(\psi_n, \mathcal{D}_p^{\otimes n}). \quad (13)$$

For  $n \leq 9$  channel uses, the optimization problem Eq. 13 is solved by *products* of repetition codes,

$$|\Phi_{\mathbf{n}}\rangle = \bigotimes_{i=1}^k |\phi_{n_i}\rangle. \quad (14)$$

Here,  $\mathbf{n} = (n_1, \dots, n_k)$ , and the resulting code  $|\Phi_{\mathbf{n}}\rangle$  is a quantum code on  $\sum_{i=1}^k n_i$  channel input qubits and  $k$  purifying qubits.

To illustrate this, consider 4 channel uses of the depolarizing channel, and recall that the single-letter coherent information Eq. 4 vanishes around  $p \simeq 0.2524$ . The respective thresholds for the 4-repetition code  $\phi_4$  and the 3-repetition code  $\phi_3$  on *three* input qubits are  $p \simeq 0.2532$  and  $p \simeq 0.2535$ , respectively (see Fig. 4 and the file `rep-codes-tabular.txt` in [Anc]). Hence, for  $0.2532 \leq p \leq 0.2535$  it is clearly advantageous to “freeze” one input qubit to some fixed pure state, and use a 3-repetition code on the remaining 3 input qubits. Since pure input states can never establish coherent information between Alice and Bob, the frozen input does not contribute to the overall

coherent information, and the resulting code incurs a penalty in the rate. However, this code inherits the same threshold as the 3-repetition code on three input qubits, thus outperforming the plain 4-repetition code. Similarly, one finds that for  $p \in [0.2519, 0.2524]$  the quantity  $\frac{1}{4}Q^{(1)}(\mathcal{D}_p^{\otimes 4})$  is maximized by a 3-repetition code tensored with a 1-repetition code (i.e., using three of the four input qubits with one purifying qubit for a repetition code, and maximally entangling the remaining input qubit with another purifying qubit). In Tab. 3 and Fig. 5, we provide an overview of the thresholds and rates of the optimal such combinations of repetition codes for  $n \leq 10$  uses of the depolarizing channel. For  $n \geq 10$  uses of the depolarizing channel, concatenated codes can surpass the best known repetition code thresholds [SS07; FW08].

$n$	$p$					
	0.25186	0.25238	0.25301	0.25329	0.25337	0.25350
4	$1 \times 3$					
5	$1 \times 1 \times 3$	$2 \times 3$	$5 \times 0$			
6	$3 \times 3$				$1 \times 5$	
7	$1 \times 3 \times 3$				$2 \times 5$	
8	$1 \times 1 \times 3 \times 3$	$2 \times 3 \times 3$	$3 \times 5$			
9	$3 \times 3 \times 3$				$1 \times 3 \times 5$	$4 \times 5$
10	$1 \times 3 \times 3 \times 3$			$5 \times 5$		

Table 3: Intermediate product repetition code thresholds; before the first column at 0.25186 the best code is given by the single-letter coherent information.

## C. Codes for the Dephrasure Channel

In the following, we give a summary of the results about the coherent information of the dephrasure channel (defined in Eq. 8) that were obtained in [LLS18a]. Superadditivity of the channel coherent information of the dephrasure channel can be achieved using a simple *weighted repetition code*

$$|\phi_n^\lambda\rangle := \sqrt{\lambda}|0\rangle_R \otimes |0^n\rangle_{A^n} + \sqrt{1-\lambda}|1\rangle_R \otimes |1^n\rangle_{A^n}, \quad (15)$$

where  $\lambda \in [0, 1]$ . In [LLS18a], the following formula is derived for its channel coherent information:

$$Q^{(1)}(\phi_n^\lambda, \mathcal{N}_{p,q}^{\otimes n}) = ((1-q)^n - q^n)h(\lambda) - (1-q)^n \left( 1 - u \operatorname{artanh} u - \frac{1}{2} \log(1-u^2) \right), \quad (16)$$

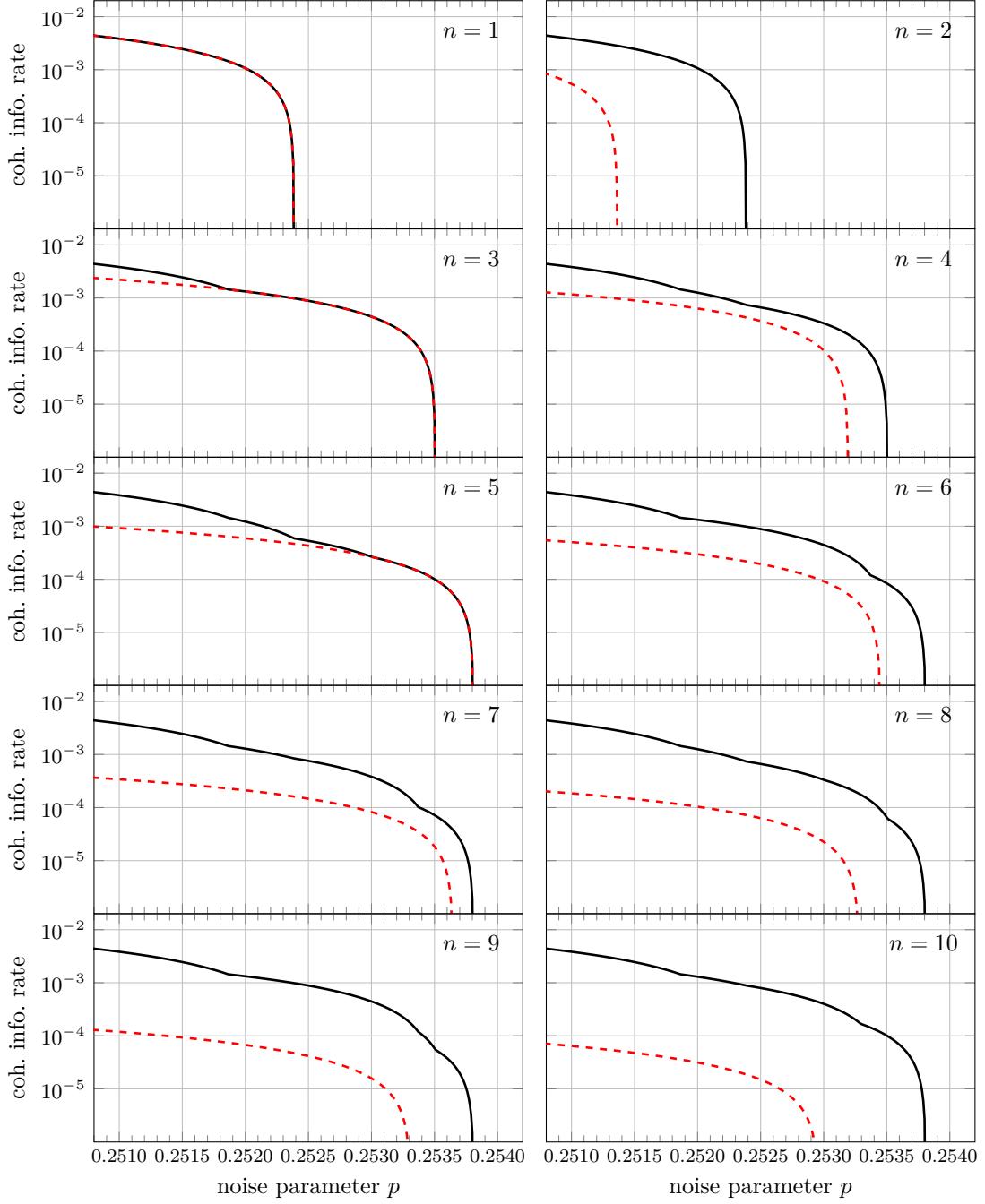


Figure 5: For  $n = 1, \dots, 10$  channel uses, the dashed red line is the coherent information rate of the  $n$ -repetition code. The solid black line is the best achievable rate when only using product codes, e.g. for  $n = 3$  and below  $p \approx 0.252$ , a product of three single-channel repetition codes ( $1 \times 1 \times 1$ ) is superior to one 3-repetition code. It is noteworthy that the segmentation of the best achievable rates is not clear *a priori*: For  $n = 4$ , the segments are  $1 \times 1 \times 1 \times 1$  and then  $3 \times 1$ , where the extra kink at  $p \approx 0.2524$  signifies that the single-letter CI has now dropped to zero; for  $n = 6$ , the segments are  $1 \times \dots \times 1$ ,  $3 \times 3$ , and  $5 \times 1$ —the latter one of which is just a single segment, as the single-letter CI is already zero.

where  $h(\lambda) = -\lambda \log \lambda - (1 - \lambda) \log(1 - \lambda)$  is the binary entropy (in terms of the binary logarithm),  $\text{artanh}(x) := \frac{1}{2} \log \frac{1+x}{1-x}$ , and

$$u = u(\lambda, p, n) = \sqrt{1 - 4\lambda(1 - \lambda)(1 - (1 - 2p)^{2n})}. \quad (17)$$

Moreover, it is shown in [LLS18a] that for  $n = 1$  the formula in Eq. 16 maximized over  $\lambda \in [0, 1]$  is in fact the optimal single-letter channel coherent information. That is,  $Q^{(1)}(\mathcal{N}_{p,q})$  is optimized by states diagonal in the computational basis. Hence, the formula Eq. 16 can be used to find quantum codes that surpass the optimal code for a single copy of  $\mathcal{N}_{p,q}$ , demonstrating superadditivity of coherent information.

In Fig. 6, we plot the optimal rates of the weighted repetition code Eq. 16 for  $n = 1, \dots, 5$  for the dephrasure channel  $\mathcal{N}_{p,3p}$  along the  $(p, 3p)$ -diagonal for  $p \in [0.107, 0.121]$ . The line corresponding to the code  $\phi_1 = \text{argmax}_\lambda Q^{(1)}(\phi_1^\lambda, \mathcal{N}_{p,3p})$  represents the optimal single-letter coherent information.

The repetition code increases the threshold for the dephrasure channel, in analogy to the case of the depolarizing channel. However, in the  $p$ -interval on the diagonal  $(p, 3p)$  where the single-letter coherent information is positive (see Fig. 6), there exist codes with higher coherent information rates, which we describe in the following.

For  $p = 0.115$ , the best known code is a code on  $k = 3$  input qubits, defined as

$$\begin{aligned} |\chi_3\rangle := & |00\rangle_R |00\rangle_{A_1 A_2} |\psi_1\rangle_{A_3} + |11\rangle_R |11\rangle_{A_1 A_2} |\psi_1\rangle_{A_3} \\ & + |01\rangle_R |01\rangle_{A_1 A_2} |\psi_2\rangle_{A_3} + |10\rangle_R |10\rangle_{A_1 A_2} X |\psi_2\rangle_{A_3}, \end{aligned} \quad (18)$$

where  $|\psi_i\rangle := c_i|0\rangle + d_i|1\rangle$ , and  $X = |0\rangle\langle 1| + |1\rangle\langle 0|$  denotes the Pauli  $X$ -operator. All coefficients above are chosen such that the code state  $\chi_3$  is normalized. Feeding the 3 right-most qubits of  $|\chi_3\rangle$  defined in eq. 18 into the 3-fold dephrasure channel  $\mathcal{N}_{p,3p}^{\otimes 3}$ , the coefficients  $c_i$  and  $d_i$  are then optimized in order to maximize the coherent information  $Q^{(1)}(\chi_3, \mathcal{N}_{p,3p}^{\otimes 3})$ . The optimal value of the coherent information for the code  $\chi_3$  is  $1.0191 \times 10^{-3}$  for  $p = 0.115$ .

For  $p = \{0.116, 0.117\}$ , the best known codes are codes on  $k = 4$  input qubits that are diagonal in the computational basis, that is, of the form

$$|\theta_4\rangle = \sum_{i^4 \in \{0,1\}^4} \lambda_{i^4} |i^4\rangle_R \otimes |i^4\rangle_{A^4}. \quad (19)$$

Optimizing the Schmidt coefficients  $\{\lambda_{i^4}\}$  with the particle swarm optimization algorithm using a ‘direct’ parametrization (as opposed to the Schmidt neural network parametrization used in the main text), the optimal values of the coherent information are  $4.6615 \times 10^{-4}$  for  $p = 0.116$  and  $1.3797 \times 10^{-4}$  for  $p = 0.117$ . Fig. 6 plots both codes  $\chi_3$  and  $\theta_4$  and compares them to the repetition codes.

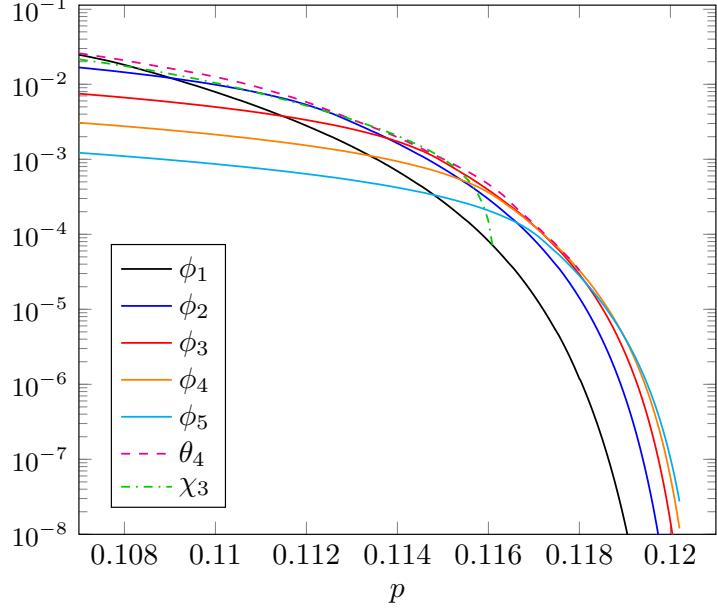


Figure 6: Plot of the known optimal codes for the dephrasure channel  $\mathcal{N}_{p,3p}$  for  $p \in [0.107, 0.121]$ . For the optimal weighted repetition codes  $\phi_n$  for  $n = 1, \dots, 5$  defined in Eq. 15, the rates were computed using the formula Eq. 16. The codes  $\chi_3$  and  $\theta_4$  are defined in Eq. 18 and Eq. 19, respectively.

As stated in the main text, we improve upon the rates resulting from the codes  $\chi_3$  and  $\theta_4$  above by finding better codes using the neural network states ansatz. More precisely, we consider  $k = 3, 4$  uses of the dephrasure channel, looking for quantum codes on  $2k$  qubits ( $k$  channel input qubits plus  $k$  purifying qubits). For  $p = 0.115$  and  $k = 3$  we find the code

$$|\nu_3\rangle = a_1(|000\rangle_R|100\rangle_{A^3} + |110\rangle_R|001\rangle_{A^3}) + a_2(|000\rangle_R|110\rangle_{A^3} + |110\rangle_R|011\rangle_{A^3}) + a_3|001\rangle_R|000\rangle_{A^3} + a_4|011\rangle_R|111\rangle_{A^3}, \quad (20)$$

where

$$\begin{aligned} a_1 &= 0.0344 + 0.0136i & a_3 &= -0.7460 + 0.2416i \\ a_2 &= -0.0012 - 0.0345i & a_4 &= -0.5657 + 0.2558i. \end{aligned} \quad (21)$$

The code  $\nu_3$  has a rate of

$$\frac{1}{3}Q^{(1)}(\nu_3, \mathcal{N}_{p,3p}^{\otimes 3}) = 1.0201 \times 10^{-3}. \quad (22)$$

For  $p = 0.116$  we find the following code,

$$\begin{aligned} |\nu_4^{(1)}\rangle &= b_1(|0000\rangle_R|0101\rangle_{A^4} + |1111\rangle_R|1010\rangle_{A^4}) \\ &\quad + b_2(|0100\rangle_R|0000\rangle_{A^4} + |1011\rangle_R|1111\rangle_{A^4}), \end{aligned} \quad (23)$$

where  $b_1 = -0.6841 + 0.1657i$  and  $b_2 = -0.0664 + 0.0161i$ . The code  $\nu_4^{(1)}$  has a rate of

$$\frac{1}{4}Q^{(1)}(\nu_4^{(1)}, \mathcal{N}_{p,3p}^{\otimes 4}) = 4.6638 \times 10^{-4}. \quad (24)$$

For  $p = 0.117$ , we find the code

$$|\nu_4^{(2)}\rangle = |0110\rangle_R \otimes (c_1|0111\rangle_{A^4} + c_2|1111\rangle_{A^4}) + c_3|1011\rangle_R|1000\rangle_{A^4}, \quad (25)$$

where  $c_1 = 0.1322 + 0.0853i$ ,  $c_2 = 0.1789 + 0.1154i$ , and  $c_3 = 0.8103 + 0.5229i$ . The code  $\nu_4^{(2)}$  has a rate of

$$\frac{1}{4}Q^{(1)}(\nu_4^{(2)}, \mathcal{N}_{p,3p}^{\otimes 4}) = 1.6401 \times 10^{-4}. \quad (26)$$

## D. Absolutely Maximally Entangled States

An AME( $n, d$ )-state is a pure state  $|\psi_{n,d}\rangle \in (\mathbb{C}^d)^{\otimes n}$  on  $n$  qudits with local dimension  $d \geq 2$  satisfying

$$\rho_{\mathcal{S}} = \text{tr}_{\mathcal{S}^c} \psi_{n,d} = \frac{1}{|\mathcal{S}|} I_{\mathcal{S}} \quad (27)$$

for every  $\mathcal{S} \subset [n]$  with  $|\mathcal{S}| = \lfloor \frac{n}{2} \rfloor$ . As mentioned in the main text, whether or not an AME( $n, d$ )-state exists depends on  $n$  and  $d$ . For example, it was proved recently in [HGS17] that an AME state on seven qubits cannot exist. However, for fixed  $n$  an AME( $n, d$ )-state always exists for sufficiently large local dimension  $d$  [HC13]. Moreover, there are constructions for certain combinations of parameters  $(n, d)$  [GBR04; HC13; Hell13; Goy+15; Goy+17]. For example, an AME( $n, d$ )-state always exists if  $d$  is a prime power and  $n \leq d$  [GBR04]. We refer to Figure 2 in [Hub+18] as well as Problem 35 on the IQOQI Vienna Open Quantum Problems list [Opq] for an overview of the known results about existence of AME( $n, d$ )-states. Here, we merely mention that it is unknown whether AME( $n, d$ )-states exist for  $(n, d) = (4, 6)$  and  $(n, d) = (7, 4), (7, 6)$ .

Scott [Sco04] proved that a multipartite state  $|\psi_{n,d}\rangle \in (\mathbb{C}^d)^{\otimes n}$  is AME if and only if the average linear entropy  $Q_m(\psi_{n,d}) = 1$ , where  $Q_m(\cdot)$  is defined in Eq. 9. Since we are searching for AME states by maximizing  $Q_m(\cdot)$ , we need to make sure that a state  $\psi_{n,d}$  with  $Q_m(\psi_{n,d}) \approx 1$  is also approximately AME. We determine the latter by introducing the average trace distance parameter  $D_m$  defined in Eq. 10 that measures the average trace distance between the marginals of  $\psi_{n,d}$  on  $m$  subsystems and the completely mixed state. The average trace distance parameter  $D_m(\cdot)$  can be bounded from above in terms of  $Q_m(\cdot)$ , as stated in Eq. 11. We restate this bound here for the reader's convenience:

$$D_m(\psi_{n,d}) \leq \sqrt{2 \log[d^m - (d^m - 1)Q_m(\psi_{n,d})]}. \quad (28)$$

To prove Eq. 28, we use the quantum version of Pinsker’s inequality,  $D(\rho\|\sigma) \geq \frac{1}{2}\|\rho - \sigma\|_1^2$ , where  $D(\rho\|\sigma) = \text{tr}(\rho \log \rho) - \text{tr}(\rho \log \sigma)$  is the quantum relative entropy. We also use the 2-relative Rényi entropy  $D_2(\rho\|\sigma) = \log \text{tr}(\rho^2 \sigma^{-1})$  [Pet86], and the well-known fact that  $D(\rho\|\sigma) \leq D_2(\rho\|\sigma)$ .

Observe first that, for  $\pi = \frac{1}{d}I$ , we have  $D_2(\rho\|\pi) = \log \text{tr}(\rho^2) + \log d$ , and hence

$$\text{tr}(\rho^2) = \frac{1}{d} \exp(D_2(\rho\|\pi)) \geq \frac{1}{d} \exp(D(\rho\|\pi)) \geq \frac{1}{d} \exp\left(\frac{1}{2}\|\rho - \pi\|_1^2\right). \quad (29)$$

Abbreviating  $\pi_{\mathcal{S}} = \frac{1}{|\mathcal{S}|}I_{\mathcal{S}}$ , we then bound

$$Q_m(\psi_{n,d}) = \binom{n}{m}^{-1} \frac{d^m}{d^m - 1} \sum_{\mathcal{S} \subset [n]: |\mathcal{S}|=m} (1 - \text{tr} \rho_{\mathcal{S}}^2) \quad (30)$$

$$\leq \binom{n}{m}^{-1} \frac{d^m}{d^m - 1} \sum_{\mathcal{S} \subset [n]: |\mathcal{S}|=m} \left(1 - \frac{1}{d^m} \exp\left(\frac{1}{2}\|\rho_{\mathcal{S}} - \pi_{\mathcal{S}}\|_1^2\right)\right) \quad (31)$$

$$= \frac{1}{d^m - 1} \left(d^m - \binom{n}{m}^{-1} \sum_{\mathcal{S} \subset [n]: |\mathcal{S}|=m} \exp\left(\frac{1}{2}\|\rho_{\mathcal{S}} - \pi_{\mathcal{S}}\|_1^2\right)\right) \quad (32)$$

$$\leq \frac{1}{d^m - 1} \left(d^m - \exp\left(\frac{1}{2}D_m(\psi_{n,d})^2\right)\right), \quad (33)$$

where the last inequality follows from concavity of the function  $x \mapsto -\exp(\frac{x^2}{2})$ . Rearranging Eq. 33 yields Eq. 28.

Since AME states are defined on tensor products of  $d$ -dimensional Hilbert spaces, the input string  $i^n$  to the neural network computing the amplitude  $\psi(i^n)$  in the ansatz Eq. 6 is a  $d$ -ary string. Depending on the local dimension, we use different encodings of this  $d$ -ary input string, as explained in E.5 below.

## E. Neural Network States

For simplicity we consider in the following a system consisting of  $n$  qubits, that is, a collection of  $n$  2-dimensional quantum systems each described by the normalized vectors in a Hilbert space isomorphic to  $\mathbb{C}^2$ . The state space of the  $n$  qudits is described by the tensor space  $(\mathbb{C}^2)^{\otimes n}$  with the “computational basis”  $\{|0\rangle, |1\rangle\}^{\otimes n}$ , and a general pure normalized quantum state  $|\psi\rangle \in \mathcal{H}^{\otimes n}$  can be written as

$$|\psi\rangle = \frac{1}{C} \sum_{i_1, \dots, i_n=0}^d \psi(i_1, \dots, i_n) |i_1\rangle \otimes \dots \otimes |i_n\rangle = \frac{1}{C} \sum_{i^n \in \{0,1\}^n} \psi(i^n) |i^n\rangle. \quad (34)$$

Here,  $C$  is a normalization constant ensuring  $\langle\psi|\psi\rangle = 1$ , the set of binary strings of length  $n$  is denoted by  $\{0,1\}^n$ , and for a string  $i^n = (i_1, \dots, i_n) \in \{0,1\}^n$  we define

$|i^n\rangle := |i_1\rangle \otimes \dots \otimes |i_n\rangle$ . Evidently, a full description of the quantum state  $|\psi\rangle$  consists of a list of the  $2^n$  complex amplitudes  $\psi(i^n)$ , corresponding to  $2 \cdot 2^n - 1$  real degrees of freedom.

For a neural network state  $\psi$ , the amplitude function  $\psi(i^n)$  in Eq. 34 is computed from the input string  $i^n$  using a neural network. There are different network architectures that can be used, and we describe a few common choices in the following subsections.

## E.1. Restricted Boltzmann States

The first architecture—and one of the most well-studied ones, see e.g. [Gla+18] for an excellent review—are restricted Boltzmann machines (RBM). They have proven particularly fruitful as a variational ansatz for representing various ground states of local Hamiltonians [CT17], notably surpassing fidelity as compared to other neural network architectures in some cases.

A Boltzmann machine has visible and hidden nodes (see Fig. 1). A set of complex variables is assigned to each node; we denote the visible units with  $i_1, \dots, i_n$ , and the hidden units with  $h_1, \dots, h_m$ . Each link between nodes corresponds to an Ising-type coupling, which defines an energy function (which one can think of as a Hamiltonian)

$$\mathbf{H}_{\text{RBM}} = \sum_{l=1}^n a_l i_l + \sum_{l=1}^m b_l h_l + \sum_{k < l} W_{kl} i_k h_l. \quad (35)$$

The two vectors  $a \in \mathbb{C}^n$  and  $b \in \mathbb{C}^m$  define a bias over the visible and hidden nodes, respectively, while the matrix  $W \in \mathbb{C}^{m \times n}$  defines the coupling between the two layers. The energy of the system allows us to define a complex probability distribution over the vectors  $i$  and  $h$  via  $\mathbb{P}(i, h) := \exp(-\mathbf{H}(i, h))/Z$  with partition function  $Z = \sum_{i, h} \mathbb{P}(i, h)$ .

To extract a weight  $\psi(i^n)$  used to assemble a state via Eq. 34, we simply trace out the hidden nodes of the RBM, which yields a marginal probability distribution over the input nodes. We obtain

$$|\psi_{\text{RBM}}\rangle = \sum_{i^n \in \{0,1\}^n} \sum_{h^n \in \{0,1\}^m} \frac{\exp(-\mathbf{H}(i^n, h^n))}{Z} |i^n\rangle. \quad (36)$$

If we take all parameters  $a, b$  and  $W$  to be real-valued, the resulting state will only have real non-negative weights. Note that as an ansatz for the depolarizing channel, code states could be assumed real due to the covariance properties of the channel, but a restriction to positive coefficients cannot be done without loss of generality.

## E.2. Deep Boltzmann States

While RBM states struggle to represent e.g. ground states for local Hamiltonians with even mildly-decaying spectral gap, adding links between the nodes within each layer yields

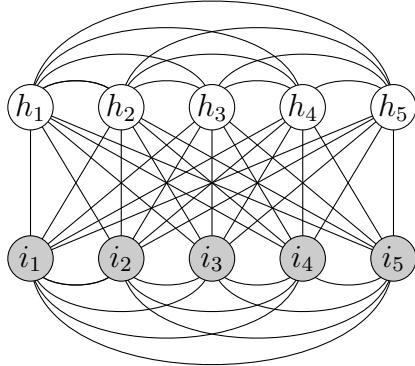


Figure 7: Deep Boltzmann machine (DBM) with five input layers, and five hidden nodes. The architecture resembles that of an RBM (see Fig. 1), but where the nodes within each layer are cross-linked. [GD17] showed that the model with connections within a layer is equivalent to one with more than two interconnected layers but no connections within each layer.

a model with vastly greater representative power [GD17; Gla+18]—deep Boltzmann machines (DBMs, see Fig. 7).

In analogy to Eq. 35, we can define an energy function for a DBM by introducing additional coupling matrices  $D \in \mathbb{C}^{m \times m}$  and  $C \in \mathbb{C}^{n \times n}$  for the hidden and visible nodes, respectively. This yields an overall Hamiltonian

$$\mathbf{H}_{\text{DBM}} = \mathbf{H}_{\text{RBM}} + \sum_{k < l} C_{kl} i_k i_l + \sum_{k < l} D_{kl} h_k h_l. \quad (37)$$

The way one obtains a state from a DBM follows the same method as for an RBM.

### E.3. Feed-Forward Network States

The third architecture is obtained by using the most prominent neural network model to date, feed-forward nets, to represent quantum states. This has proven successful in a number of cases [CL18; Sai17].

A feed-forward network consists of a visible layer  $v = i^n$  with input nodes  $i_1, \dots, i_n$ , a fixed number  $H$  of hidden layers  $h^{(j)}$  of width  $M_j$ , and an output layer  $o$  with two output nodes  $o_1$  and  $o_2$  (see Fig. 1). Each hidden neuron  $h_k^{(j)}$  for  $j \in [H]$  and  $k \in [M_j]$  is assigned a *bias*  $b_k^{(j)}$ , and the interactions between two hidden layers  $h^{(j-1)}$  and  $h^{(j)}$  are mediated by *weight matrices*  $(W_{kl}^{(j)})_{kl}$  where  $k \in [M_j]$  and  $l \in [M_{j-1}]$ . The weight matrix  $W^{(1)}$  mediates between the visible layer and the first hidden layer, and the weight matrix  $W^{(H+1)}$  mediates between the last hidden layer  $h^{(H)}$  and the output layer  $o$ .

with bias  $b^{(H+1)}$ . In each hidden layer  $h^{(j)}$  the state of the neurons is processed with a non-linear activation function  $f_j$ . In the following, we interpret the visible layer  $v$ , the hidden layers  $h^{(j)}$ , and the output layer  $o$  as column vectors, and functions are evaluated component-wise. Given the input  $v = i^n$ , the amplitude function  $\psi(i^n)$  is computed as follows:

$$\begin{aligned} h^{(1)} &= f_1 \left( W^{(1)}v + b^{(1)} \right) \\ h^{(j)} &= f_j \left( W^{(j)}h^{(j-1)} + b^{(j)} \right) \quad \text{for } j = 2, \dots, H \\ o &= W^{(H+1)}h^{(H)} + b^{(H+1)} \end{aligned} \tag{38}$$

Cartesian:  $\psi(i^n) = o_1 + io_2$

Polar:  $\psi(i^n) = \exp(o_1 + io_2)$ .

A network architecture is specified by the data  $(H, \{M_j, f_j\}_{j \in [H]})$ . Common choices for the activation functions are the sigmoid function  $\sigma(x) := (1 + \exp(-x))^{-1}$ , the hyperbolic tangent tanh, or the rectified linear unit  $\text{ReLU}(x) = \max\{0, x\}$  (see Sec. 8). From a theoretical point of view these choices are all equivalent, since feed-forward networks as described above are *universal*: With a single hidden layer, they can approximate any given function to arbitrary precision provided the activation function is non-constant and the number of hidden neurons is sufficiently large [Kol61; Hor91]. However, in practice the choice of activation functions has to be tailored to the problem at hand to achieve good numerical results. In Sec. E.6, we elaborate on the heuristics of choosing activation functions for neural network states; of particular interest in this context is that periodic activation functions—such as  $\cos$ —seem to be able to capture more of the structure of various quantum states [CL18]. We prove analytically in App. F that periodic activation functions are also beneficial in representing good quantum codes.

## E.4. Schmidt Network States

A slightly modified proposal from feed-forward and RBM network states in Eq. 34 are Schmidt networks, where instead of calculating the full state vector with a neural net, we take the network output to represent the Schmidt weights with respect to, e.g., the computational tensor basis:

$$|\psi\rangle = \frac{1}{C} \sum_{i^n \in \{0,1\}^n} \psi(i^n) |i^n\rangle |i^n\rangle. \tag{39}$$

This ansatz obviously introduces a choice of basis; we note, however, that the channel coherent information in Eq. 3 is invariant under unitary transformations which do not cross between system and environment. The Schmidt ansatz further allows the network to only have real parameters, since Schmidt coefficients are real by definition.

## E.5. Input Encoding of $d$ -ary Strings for Neural Networks

In order to parametrize quantum states on  $n$  qubits, it is rather straightforward to use the neural network ansatz described in the main text and App. E. In the case of AME( $n, d$ )-states with local dimension  $d > 2$ , we slightly tweak the neural network ansatz. To this end, we fix a basis  $\{|i\rangle\}_{i=0}^{d-1}$  for  $\mathbb{C}^d$ , and express a general quantum state  $\psi_{n,d} \in (\mathbb{C}^d)^{\otimes n}$  as

$$|\psi_{n,d}\rangle = \frac{1}{C} \sum_{i^n \in [d]_0^n} \psi(i^n) |i^n\rangle, \quad (40)$$

where  $C$  is again a normalization constant ensuring  $\langle \psi_{n,d} | \psi_{n,d} \rangle = 1$ , and we use the notation  $[d]_0 := \{0, \dots, d-1\}$ . We consider three different options of encoding the  $d$ -ary input string  $i^n$  in order to obtain the amplitudes  $\psi(i^n)$  in Eq. 40 from a neural network:

1. (Scaled) direct encoding: Use the  $d$ -ary string  $i^n$  directly, with a possible scaling of the entries such that  $i_k \in [0, 1]$  for  $k \in [n]$ .
2. Binary encoding: Convert each symbol  $i_k \in [d]_0$  into a binary string, requiring  $\lceil \log d \rceil$  ‘physical’ qubits per ‘logical’ qudit of  $\psi_{n,d}$ , and use the resulting binary string of length  $\lceil \log d \rceil n$  as the input to the neural network.

Example: For  $d = 6$ , the encoding is  $0 \mapsto 000, 1 \mapsto 111, \dots, 5 \mapsto 101$ .

3. One-hot encoding: Encode each symbol in a ‘one-hot’ vector of length  $d$  and use the resulting binary string of length  $dn$  as the input to the neural network.

Example: For  $d = 6$ , the encoding is  $0 \mapsto 000001, 1 \mapsto 000010, \dots, 5 \mapsto 100000$ .

We have found that the performance of the specific encoding used in the neural network optimization depends on the local dimension  $d$ . For prime  $d$ , the neural network optimization using the scaled encoding converges quickly to known AME( $n, d$ )-states such as AME(4, 7) (see Fig. 3 in the main text). On the other hand, for composite  $d$  the NN ansatz is more powerful using one of either the binary encoding or the one-hot encoding. Since binary encoding has a smaller overhead in terms of the ‘physical’ qubits used in the ansatz ( $\lceil \log d \rceil n$  vs.  $dn$ ), we use binary encoding for composite local dimension  $d$ . We summarize the different encodings in Tab. 4.

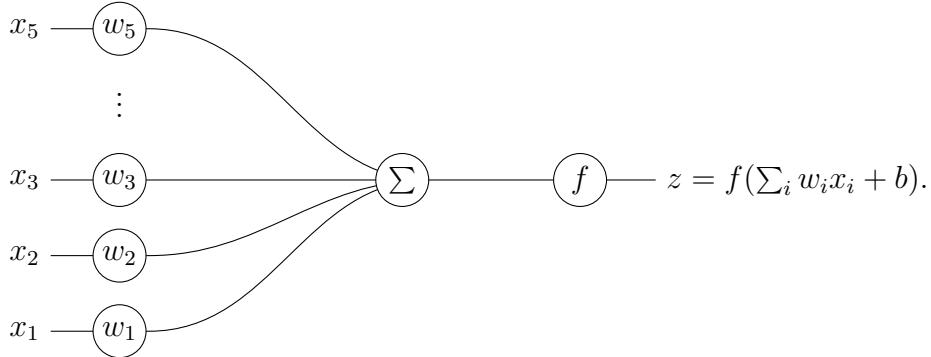
## E.6. The Role of Activation Functions for Quantum Codes

In machine learning, the use of nonlinear activation functions is crucial to a neural network’s performance—since otherwise the network is just a single affine transformation, not useful beyond linear regression. The overall network can have varying activation

	encoding ( $i \in [d]_0$ )	# input nodes
scaled	$i \mapsto i/(d-1)$	$n$
binary	$i \mapsto \text{bin}_{\lceil \log d \rceil}(i)$	$\lceil \log d \rceil n$
one-hot	$i \mapsto e_i$	$d n$

Table 4: Summary of the possible encodings of a symbol  $i \in [d]_0$  in a  $d$ -ary string  $i^n$  of length  $n$ . We denote by  $\text{bin}_k(m)$  the binary representation of  $m$  of length  $k$  (with leading zeros if necessary), and by  $e_i$  a vector with a 1 in the  $i$ -th component and 0s elsewhere.

functions per neuron (see Fig. 1); in essentially all cases, the activation functions are the same within a layer. The operation of such a layer is thus to perform an affine transformation on the input vector and then, element-wise, apply the nonlinearity  $f$ . For a single neuron  $z$  depending on  $x = (x_1, \dots, x_n)$ , the mathematical operation can thus be visualized as



Commonly used activation functions are e.g. ReLU, sigm or tanh, which are plotted in Fig. 8; in addition to some thorough studies [IS15; He+15; KSH17], there seems to be a lot of empirical understanding which activation functions perform better in various scenarios [der]. One example is that e.g. sigm saturates (meaning the gradient vanishes for large or small values), whereas e.g. ReLU does not have the same problem. Furthermore, the general consensus seems to be that non-monotonic or periodic activation functions—such as e.g. sin—weaken the neural network’s performance. We found conflicting evidence for this in the literature ([Sop99; GA16] and [GBC16, sec. 6.2.2]), suggesting that such periodic functions can indeed be useful for specific tasks—especially in the context of representing ground states for local Hamiltonians [CL18].

In one example of such a task, [CL18] use neural network states to approximate the ground states of certain Hamiltonians. They report good performance of feed-forward network architectures with a cosine activation function in the first layer for a 1D anti-ferromagnetic Heisenberg model, arguing that the cosine function is capable of handling

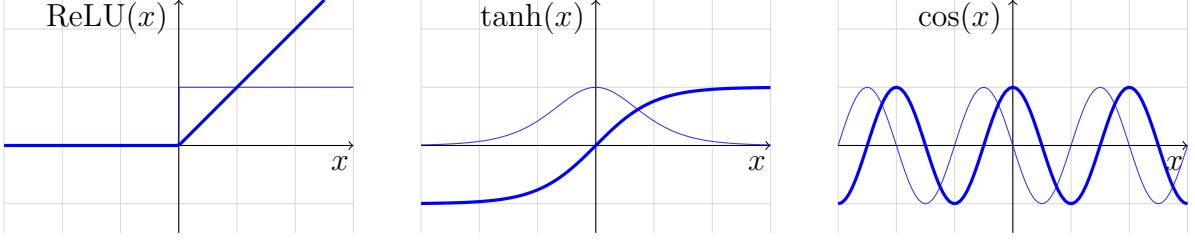


Figure 8: Various activation functions (bold lines) and their derivatives (thin lines).  $\tanh(x)$  is an example for a sigmoid function; more commonly used, however, is  $\text{sigm}(x) = (1 + \exp(-x))^{-1}$ . It is clear that sigmoid functions suffer from a vanishing gradient problem on both ends of its input. This can be countered either by going to another activation function—such as a rectified linear unit  $\text{ReLU}$  (or its “leaky” version, i.e. one where the segment for  $x < 0$  has a small but non-vanishing slope), or using techniques such as batch normalisation [IS15]. Non-monotonic activation functions such as  $\cos$  are rarely used in practice, but can be useful for certain specific tasks.

the “sign problem” typically found in the analysis of Hamiltonians. We found that using cosine in the first hidden layer also performs well in finding good quantum codes for quantum channels such as the depolarizing channel defined in Eq. 1, or the dephrasure channel defined in Eq. 8.

In the following, we want to give an intuition why a periodic activation function such as  $\cos$  can be useful for learning quantum codes with a structure that can be easily derived from the binary signature of its state vector. To give an example, consider a repetition code on five qubits, given by  $|00000\rangle + |11111\rangle$ . A function  $M: (\mathbb{C}^2)^{\otimes 5} \rightarrow \mathbb{C}$  with  $M(|00000\rangle) = M(|11111\rangle) = 1$ , and 0 elsewhere, is trivial to construct from elementary logic gates (i.e. either all bits are zero, or all bits are one).

For a feed-forward neural network, one could imagine adding up all bits within one neuron, and thresholding this value with a  $\text{ReLU}$  activator:

$$z_1 = \text{ReLU}\left(2 \sum_{i=1}^5 x_i - 9\right) = \begin{cases} 1 & \text{if } x_i = 1 \forall i \\ 0 & \text{otherwise.} \end{cases}$$

A similar gate with flipped signs can activate only when all bits are zero; the two outputs can then be combined using a final  $\text{ReLU}$  node.

We can achieve the same activation using a single  $\cos$  neuron, dovetailed by a  $\text{ReLU}$  in the next layer:

$$z_1 = \cos\left(\frac{2\pi}{5} \sum_{i=1}^5 x_i\right) \quad \text{and} \quad z_2 = \text{ReLU}\left(\frac{z_1 - \cos(1/5)}{1 - \cos(1/5)}\right).$$

While this looks like a more complicated version of the same calculation, it quickly becomes obvious that one can easily perform modular arithmetic using this technique—what we have in fact calculated is whether  $\sum_i x_i \equiv 0 \pmod{5}$ .

Why is this an advantage? As a slightly more complicated example, let us consider an (unnormalized) tensor code built from a 3-repetition code  $|\phi_3\rangle = |000\ 000\rangle + |111\ 111\rangle$  and a 1-repetition code (or simply maximally entangled state)  $|\phi_1\rangle = |0\ 0\rangle + |1\ 1\rangle$ . In both cases, the first block of qubits (3 resp. 1) is sent through the channel, and the second block form the purifying environment. On 4 qubits, the tensor code thus looks as follows (for visualization purposes we boldface the single channel repetition code):

$$|\phi_3\rangle \otimes |\phi_1\rangle = |\mathbf{0}000\ 0000\rangle + |\mathbf{0}001\ 0001\rangle + |\mathbf{1}110\ 1110\rangle + |\mathbf{1}111\ 1111\rangle \quad (41)$$

Any tensor channel  $\mathcal{N}^{\otimes n}$  is naturally covariant<sup>3</sup> with respect to permuting tensor factors, i.e., the unitary representation  $\pi \mapsto U_\pi$  of the symmetric group  $S_n$  on  $(\mathbb{C}^2)^{\otimes n}$  defined by  $U_\pi|e_1\rangle \otimes \dots \otimes |e_n\rangle = |e_{\pi^{-1}(1)}\rangle \otimes \dots \otimes |e_{\pi^{-1}(n)}\rangle$ . Since the coherent information  $I(A)B$  is furthermore invariant under local unitaries of the form  $U_A \otimes U_B$ , codes that are permutations of each other yield the same value for the coherent information. For example, the code

$$(U_{(14)} \otimes U_{(24)})(|\phi_3\rangle \otimes |\phi_1\rangle) = |\mathbf{0}000\ 0000\rangle + |\mathbf{1}000\ 0100\rangle + |\mathbf{0}111\ 1011\rangle + |\mathbf{1}111\ 1111\rangle \quad (42)$$

is obtained from  $|\phi_3\rangle \otimes |\phi_1\rangle$  by swapping channel qubits 1 and 4 and environment qubits 2 and 4,<sup>4</sup> and is thus equivalent for quantum information transmission.<sup>5</sup> Hence, within each block of four qubits (either channel or environment) the code is characterized by the Hamming weight of the code vectors (0, 1, 3 and 4 in the example above), and ideally this is identified by the neural network. With modular arithmetic, we can have a cos neuron identifying 0 and 4 (e.g. all Hamming weights  $\equiv 0 \pmod{4}$ ), and another one 1 and 3 (e.g. all odd Hamming weights).

While it is conceivable that for simple codes such as Eq. 41 one can write down relatively simple circuits with non-periodic activation functions, it should be clear that we do save space within the neural network if we can perform calculations such as the ones above within a single node.

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<sup>3</sup>A quantum channel  $\mathcal{M}: A \rightarrow B$  is *covariant* with respect to a group  $G$  if there are unitary representations  $g \mapsto U_A(g)$  on  $\mathcal{H}_A$  and  $g \mapsto U_B(g)$  on  $\mathcal{H}_B$  such that  $\mathcal{M}(U_A(g) \cdot U_A(g)^\dagger) = U_B(g)\mathcal{M}(\cdot)U_B(g)^\dagger$  for all  $g \in G$ .

<sup>4</sup>Note that in Eq. 42 the two tensor products on the left-hand side are with respect to different tensor factors. For the first tensor product, the two factors correspond to channel input and purifying qubits, respectively.

<sup>5</sup>We do *not* claim that optimal codes are in any way symmetric due to this permutation invariance.

## F. Products of Repetition Codes as Benchmark

As a benchmark for finding quantum codes, we demand that the models we propose can at least achieve the product repetition codes described above; either because they can represent products of repetition codes directly, or because they achieve the target rates by some other means. In particular, this should serve as a sanity check for the models we propose, indicating whether we need to increase the width of a hidden layer, or the depth of the model. The relevant question for us is whether a state  $|\Phi_n\rangle$  as defined in Eq. 14 can always be represented accurately by the weights obtained from an RBM or an FF net.

### F.1. RBM States

First observe how the Hamiltonian  $\mathbf{H}_{\text{RBM}}$  describes a linear single-layer FF classifier (i.e., a linear function on the inputs  $i_k$ ). Seen as a linear function on bit strings, the Hamiltonian can therefore represent a target state  $|\psi\rangle$  as well as a linear model allows. For the simple case of products of repetition codes, where we subdivide the set of basis states into those of weight 0 and 1, respectively, this question is well-studied in the context of linear classifiers.

A single  $k$ -repetition code has the form  $|0 \cdots 0\rangle + |1 \cdots 1\rangle =: |a\rangle + |b\rangle$ . Since the RBM uses a scaled encoding (see Tab. 4), the bit strings correspond to real entries in a  $k$ -dimensional vector, and thus  $|b\rangle = 0|a\rangle$ ; a linear function  $L$  therefore necessarily satisfies  $L(|b\rangle) = L(|a\rangle) = 0$ . If we let  $|b\rangle$  be a basis state (unnormalized) and complete the basis with  $k - 1$  arbitrary orthogonal vectors, it therefore suffices to define  $L$  in such a way to have  $\ker L = \text{span}\{|b\rangle\}$ .

Products of repetition codes always have the form  $\bigotimes_{i=1}^k |\phi_{n_i}\rangle$ ; since basis states are bit strings for the RBM classifier, the corresponding code is a direct sum of the individual repetition codes. We can thus construct a classifier for the overall code by writing  $L_1 \oplus \dots \oplus L_k = L$ , which is still linear.

Since  $\mathbf{H}_{\text{RBM}}$  appears in an exponential in Eq. 36, we can use the spectral gap of  $\mathbf{H}_{\text{RBM}}$  to obtain a lower bound on how close to zero an entry in the code can be set. For instance, if we were to represent a 3-repetition code  $|000\rangle + |111\rangle$ , we can require that  $|111\rangle$  is the eigenvector corresponding to the smallest eigenvalue of  $\mathbf{H}_{\text{RBM}}$ ; all other binary strings should have an energy that is as large as possible, such that the exponential function suppresses the corresponding weight. Consider the binary state  $|011\rangle$ , which has overlap  $\sqrt{2/3}$  with  $|111\rangle$  (assuming normalization). If  $\Delta$  is the spectral gap of  $\mathbf{H}_{\text{RBM}}$ —i.e. the difference between the ground state energy and the second lowest eigenvalue—then  $\langle 001| \mathbf{H}_{\text{RBM}} |001\rangle = 2\Delta/3$ , yielding a lower bound between largest code

weight and smallest code weight of  $\exp(-\Delta)$ . To get an empirical estimate, assume we flip a single bit—e.g.  $i_1$ —in Eq. 35. How large can the energy difference be? If all parameters are chosen (in magnitude) within a range  $[-M, M]$ , then a simple estimate would be  $\Delta \leq M + M^2$ ; this is, of course, an upper bound to a lower bound. In practice we found that  $M = 10$  is sufficient for our purposes.

## F.2. DBM States

Eq. 37 introduces a quadratic term in the input. Since one can easily embed a 1-IN-3SAT instance into a quadratic polynomial (for three boolean variables  $v_1, v_2, v_3$  where **TRUE**=1 and **FALSE**=0 enforced by terms  $v_i^2 - v_i = 0$ , the equation  $(v_1 + v_2 + v_3 - 1)^2 = 0$  if and only if exactly one of the  $v_i$  is **TRUE**; the existence or nonexistence of a root for the sum of all constraints thus answers the instance), it is clear that the discriminative power of DBM states should vastly outperform that of RBM states, albeit at a higher computational cost. As discussed in the introduction, for various ground states of local Hamiltonians this intuition has empirically been shown to be correct.

## F.3. Feed Forward Network States

It is easy to explicitly construct weights for an FF net that can represent any product repetition code. As a first step, consider a single repetition code  $|\phi_n\rangle$ . We set up a three-layer neural network from  $n$  inputs, one hidden layer of width 1, and a single output node (for simplicity we disregard the imaginary part for the state output in Eq. 38). The weights and activation functions to be chosen are

$$\{x_i\}_{i=1}^{n+1} \longmapsto y := \cos\left(\frac{2\pi}{n+1} \sum_{i=1}^{n+1} x_i\right) \longmapsto z := \text{ReLU}\left(\frac{y - \cos(2\pi/n+1)}{1 - \cos(2\pi/n+1)}\right), \quad (43)$$

and one can verify that the output is one on the all 1s and 0s input, and zero otherwise. We refer to Sec. E.6 for a more detailed discussion.

For a product code given by some  $\mathbf{n} = (n_1, \dots, n_k)$ , we simply partition the input nodes into  $k$  subsets and dovetail those with a network given in Eq. 43; we obtain  $k$  outputs  $z_1, \dots, z_k$ . Since we know that a logic AND gate corresponds to all the  $z_i = 1$ , we can use a final  $\text{ReLU}(\sum_{i=1}^k z_i - k + 1)$  layer to enforce that the weights are 1 if all individual segments are valid repetition codes, and 0 otherwise—or merge all already existing ReLU nodes into one. Observe that we could always implement a single cos node in this function with two ReLU nodes, followed by another ReLU node to combine the outputs (as in Sec. E.6). This would increase the hidden layer width by a factor of two; we can incorporate addition of the individual outputs into the last existing ReLU layer, so the depth should remain constant.

One immediate consequence is that any product code of  $k$  repetition codes can always be represented by a network architecture where the first hidden layer has width  $k$ ; and we in fact empirically found that the trained weights of the first layer are similar to those in Eq. 43.

A final note on the parameter range necessary for the argument: the largest coefficients in absolute value in Eq. 43 and its final AND node are  $\max_i(1 - \cos(2\pi/n(i)))^{-1}$ , or  $k - 1$ , whichever is larger. Restricting the network's parameter range artificially below this threshold could result in worse representability of product repetition codes.

#### F.4. Schmidt Network States

The argument is similar as for feed-forward network states; note that, in general, Schmidt codes will be redundant since for e.g. four channel uses, we are forced to using more than just a single purifying qubit. The fact that the neural net calculates Schmidt coefficients means that the repetition codes always uses as many purifying dimensions as system dimensions.

### G. Numerical Optimization Techniques

In most applications neural networks are trained using the backpropagation method, in which each network parameter is updated using the gradient of a loss or objective function with respect to that parameter. In our main application of neural networks, maximizing the coherent information of a quantum channel, the objective function is the coherent information itself. In the interesting case of a high-noise quantum channel (such as  $\mathcal{D}_p$  for  $p \gtrsim 0.2523$ ), a randomly selected quantum code (e.g., with respect to the Haar measure on pure states) has strictly negative coherent information with high probability, whereas a product state  $|\psi_1\rangle_R \otimes |\psi_2\rangle_A$  always has vanishing coherent information,  $I_c(\psi_1 \otimes \psi_2, \mathcal{N}) = S(\mathcal{N}(\psi_2)) - S(\psi_1 \otimes \mathcal{N}(\psi_2)) = 0$ . Hence, the coherent information landscape is dominated by local maxima, and gradient-based optimization techniques are likely to get stuck in these local maxima.

This intuition was confirmed in our numerical search for good quantum codes for the depolarizing channel and the dephrasure channel. In the search for  $\text{AME}(n, d)$  states, the objective function is the function  $Q_m(\psi)$  defined in Eq. 9. Here, numerical investigations also showed that gradient-based optimization was again likely to get stuck in local minima.

The failure of gradient-based optimization methods in both scenarios led us to consider gradient-free, stochastic global optimization techniques instead. In the following, we give high-level explanations of four popular such algorithms, particle swarm optimization,

artificial bee colonization, pattern search (also known as direct search), and genetic evolution.

## G.1. Particle Swarm Optimization

*Particle swarm optimization* (PSO) [KE95] is a meta-heuristic, derivative-free global optimization technique. The idea of PSO is to have multiple *particles* explore the landscape on the search for a global minimum, and communicate their individual best value to the swarm. At the same time, each particle records its own history and stores the personal best value. In each iteration, the update of a particle's velocity vector is determined by the current velocity, recurrence to the location of the personal best function value, and attraction towards the location of the global best value.

More precisely, fix model parameters  $\alpha, \beta, \gamma > 0$  and consider  $N$  particles with random initial position  $\mathbf{x}_i^{(0)}$  and random initial velocity  $\mathbf{v}_i^{(0)}$  for  $i \in [N]$ . For each particle  $i$ , the variable  $\mathbf{p}_i$  stores the location of the personal best function value, while the variable  $\mathbf{g}$  stores the location of the global best function value among the whole swarm. In the  $k$ -th iteration, the velocity and position of a particle are updated according to

$$\mathbf{v}_i^{(k)} = \alpha \mathbf{v}_i^{(k-1)} + \beta r_\beta (\mathbf{p}_i - \mathbf{x}_i^{(k-1)}) + \gamma r_\gamma (\mathbf{g} - \mathbf{x}_i^{(k-1)}) \quad (44)$$

$$\mathbf{x}_i^{(k)} = \mathbf{x}_i^{(k-1)} + \mathbf{v}_i^{(k)}, \quad (45)$$

where  $r_\beta, r_\gamma \in [0, 1]$  are drawn uniformly at random. The parameter  $\alpha$  is called *inertia*, while  $\beta$  and  $\gamma$  are usually called *self-interaction* and *social interaction*, respectively. A common modification of the particle swarm optimization is to limit the social interaction to neighborhoods of a certain size within the swarm, ensuring a more thorough exploration of the landscape by the swarm.

The MATLAB implementation of PSO, available in the Global Optimization Toolbox, uses the neighborhood modifications with variable neighborhood sizes and an adaptive adjustment of the inertia weight. We refer to the official documentation [Pso] for details of the algorithm, as well as the MATLAB files in [Anc] for the algorithm settings used in this paper. Furthermore, we used the “inertia weight” variant of PSO in Pagmo [Abc], with parameter settings as found in the C++ source files [Anc].

## G.2. Artificial Bee Colonization

*Artificial bee colonization* (ABC) [Kar05] is another meta-heuristic, derivative-free global optimization technique based on the principle of swarm intelligence. The algorithm works as follows: The population consists of  $N$  employer bees and  $N$  onlooker bees. While the employer bees explore the neighborhood of randomly created ‘food sources’ (i.e., points

in the landscape with a low objective function value), the onlooker bees evaluate the food sources according to the promise given by the *fitness* of the food source, and join the employer bees in exploring the neighborhood of those food sources. If an employer bee cannot find any new food around its location for a certain number of iterations (i.e., it fails to find points in the neighborhood of the food source with a lower objective function value), it is converted into a *scout bee* and assigned to a new random food source.

In more detail, to minimize a function  $f: \mathbb{R}^D \rightarrow \mathbb{R}$ , an employer bee at site  $x_i$  randomly explores the neighborhood of  $x_i$  by probing the location  $x'_i$  which differs from  $x_i$  in exactly one randomly drawn component  $j \in [D]$  according to

$$(x'_i)_j = (x_i)_j + r((x_i)_j - (x_k)_j), \quad (46)$$

where  $x_k \neq x_i$  is another randomly drawn food source, and  $r \in [-1, 1]$  is a uniform random number. If  $f(x'_i) < f(x_i)$ , the employer bee switches to  $x'_i$  and continues exploring its neighborhood. The fitness of the food source  $x_i$  is defined as  $\text{fit}_i := (1 + f(x_i))^{-1}$ , and each onlooker bee reinforces the employer bee group by selecting a food source according to the probability distribution  $\{\text{fit}_i / \sum_i \text{fit}_i\}_i$ .

We use the standard implementation of ABC found in the C++ optimization library Pagmo [[Abc](#)], as well as our own implementation of the standard algorithm in MATLAB (see [[Anc](#)]).

### G.3. Pattern Search

The third derivative-free optimization technique we use in this paper is called *pattern search* or *direct search*. To minimize a function  $f: \mathbb{R}^D \rightarrow \mathbb{R}$ , the algorithm takes as input a starting point  $x_0 \in \mathbb{R}^D$  together with the objective function value  $f(x_0)$ , and creates a mesh of probing points around the starting point. In each iteration or *poll*, the objective function is evaluated at each mesh point. If for one of the mesh points, say  $x_1$ , the objective function value is lower than the current one (at  $x_0$ ), the algorithm centers at  $x_1$  and creates a new mesh.

There are different ways in how the mesh at a new center point is created. In a popular variant called *generalized pattern search* (GPS), the new probing points  $y_i$  of the mesh are defined by a fixed set  $\mathcal{S} \subset \mathbb{R}^D$  of vectors. Common choices are  $\mathcal{S}_{2D} = \{\pm \mathbf{e}_i\}_{i=1}^D$ , where  $\mathbf{e}_i$  denotes the  $i$ -th standard basis vector, or  $\mathcal{S}_{D+1} = \{\mathbf{e}_i\}_{i=1}^D \cup \{-(\mathbf{e}_1 + \dots + \mathbf{e}_D)\}$ . In the  $k$ -th round with center point  $x_{k-1}$ , the points of the mesh are defined as  $y_i = x_{k-1} + \Delta v_i$ , where  $v_i \in \mathcal{S}$ , and  $\Delta$  is the *mesh constant*. In a successful poll (i.e., when a new point with a lower objective function value is found), the mesh constant for the new mesh is doubled. If the poll is unsuccessful, the center point remains the same and  $\Delta$  is halved.

Another popular variant is called *mesh adaptive direct search* (MADS). Here, the set  $\mathcal{R} \subset \mathbb{R}^D$  of vectors for the new mesh points is randomly created after each successful poll. In analogy to the GPS variant above, common choices are  $\mathcal{R}_{2D} = \{\pm \mathbf{v}_i\}_{i=1}^D$  and  $\mathcal{R}_{D+1} = \{\mathbf{v}_i\}_{i=1}^D \cup \{-(\mathbf{v}_1 + \dots + \mathbf{v}_D)\}$ , where in each case the  $\mathbf{v}_i$  are random vectors.

The above variants of pattern search are available in the Global Optimization Toolbox of MATLAB [Psm]. We refer to the MATLAB files in [Anc] for the algorithm settings used in this paper.

## G.4. Simple Genetic Algorithm

The fourth derivative-free optimization algorithm is a genetic algorithm, which is related to evolutionary methods such as PSO and ABC, but motivated from the process of gene evolution.

Starting from a random selection of  $N$  so-called “chromosomes”  $\mathbf{x}_i^{(0)}$ —where each vector component is called a “gene”—a traditional implementation follows four steps.

**Selection.** Pick random tuples of size  $s$  from the chromosome pool, and select the ones with the best function value within each tuple; this creates a selected chromosome pool of size less than  $N$ .

**Crossover.** Randomly select a parent tuple (can be more than two, and up to the entire selected pool). Merge the parents, e.g. by selecting a random chromosome, and replacing each gene (coordinate of  $\mathbf{x}_i^{(0)}$ ) with some probability  $p$  by genes from other chromosomes. Continue creating child chromosomes until the new pool reaches size  $N$ .

**Mutation.** Randomize child genes within each chromosome according to some randomness distribution  $\mathcal{D}$  and mutation probability  $m$ ; a popular variant of which is called *polynomial mutation* where  $\mathcal{D} \sim 1/\text{poly}$ , which introduces a stronger bias towards creating children close to their parents.

**Reinsertion.** Merge parent and child chromosome pool and select  $N$  of the fittest candidates.

We use Pagmo’s standard implementation of a simple genetic algorithm with polynomial mutation (SGE, [Sge]), with parameters  $s = 2$ ,  $p = 0.9$  and  $m = 0.02$ .

## H. Additional Numerical Data

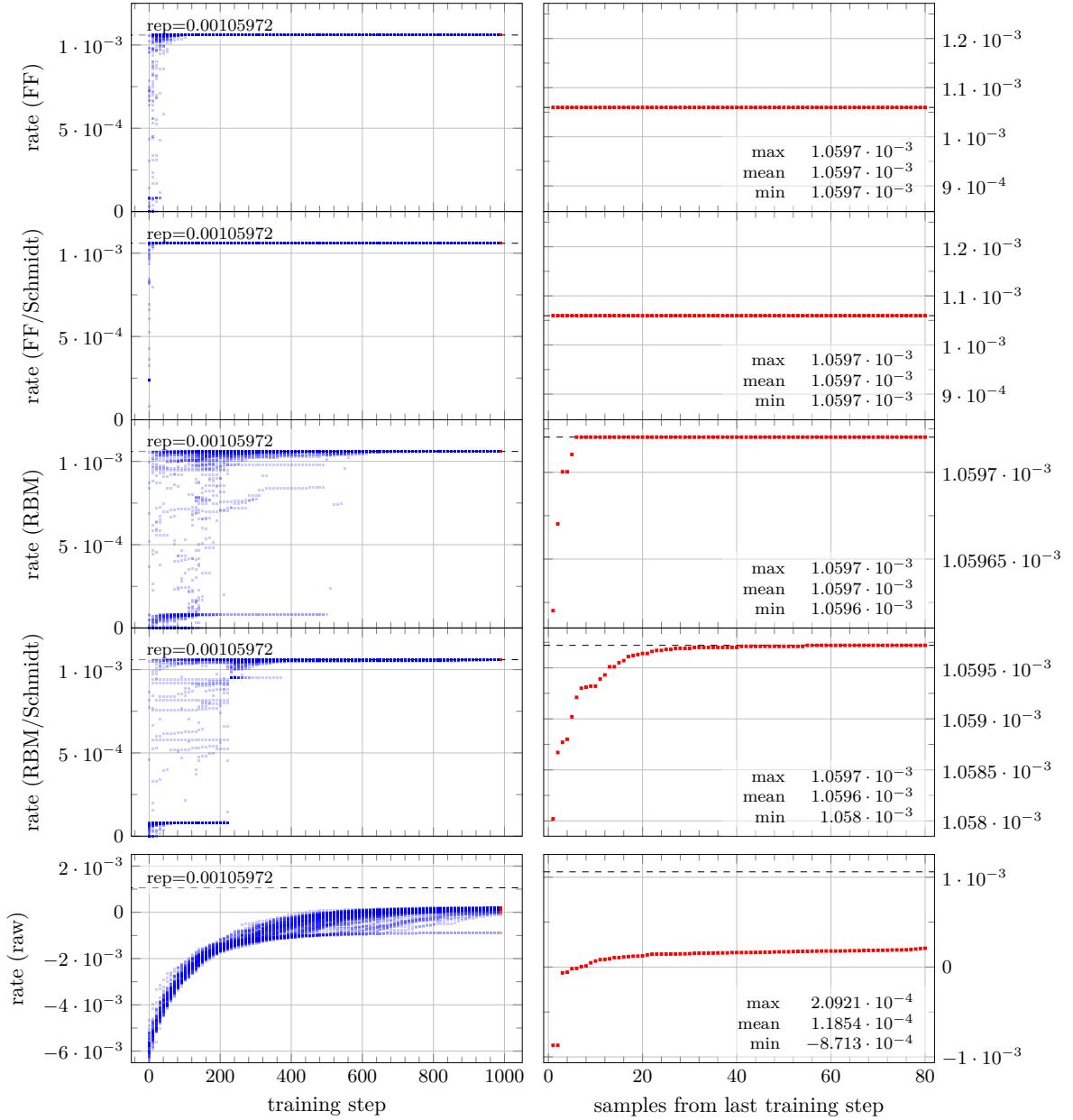


Figure 9: Training convergence of an artificial bee colony (ABC) algorithm implemented in pagmo, maximizing the CI of three copies of the depolarizing channel  $\mathcal{D}_p$ , with noise parameter  $p = 0.2523$ . The network architectures are identical to the ones in Fig. 2.

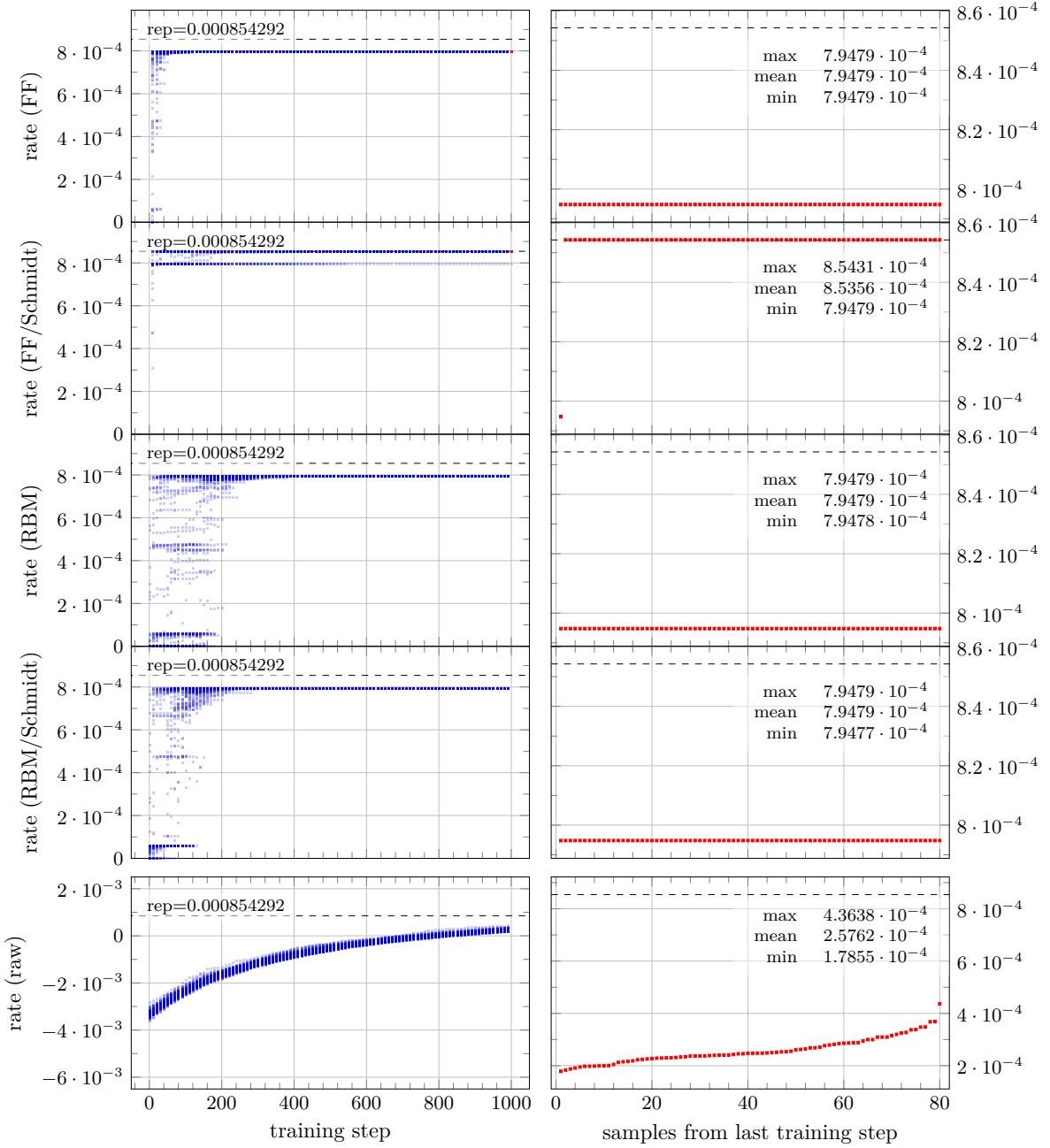


Figure 10: Training convergence of an artificial bee colony (ABC) algorithm implemented in pagmo, maximizing the CI of four copies of the depolarizing channel  $\mathcal{D}_p$ , with noise parameter  $p = 0.2523$ . The network architectures are identical to the ones in Fig. 2. We remark that ABC seems to have troubles moving beyond a local minimum around the three-repetition code with  $\text{CI} = 0.0007948$  in all but the FF/Schmidt ansatz.

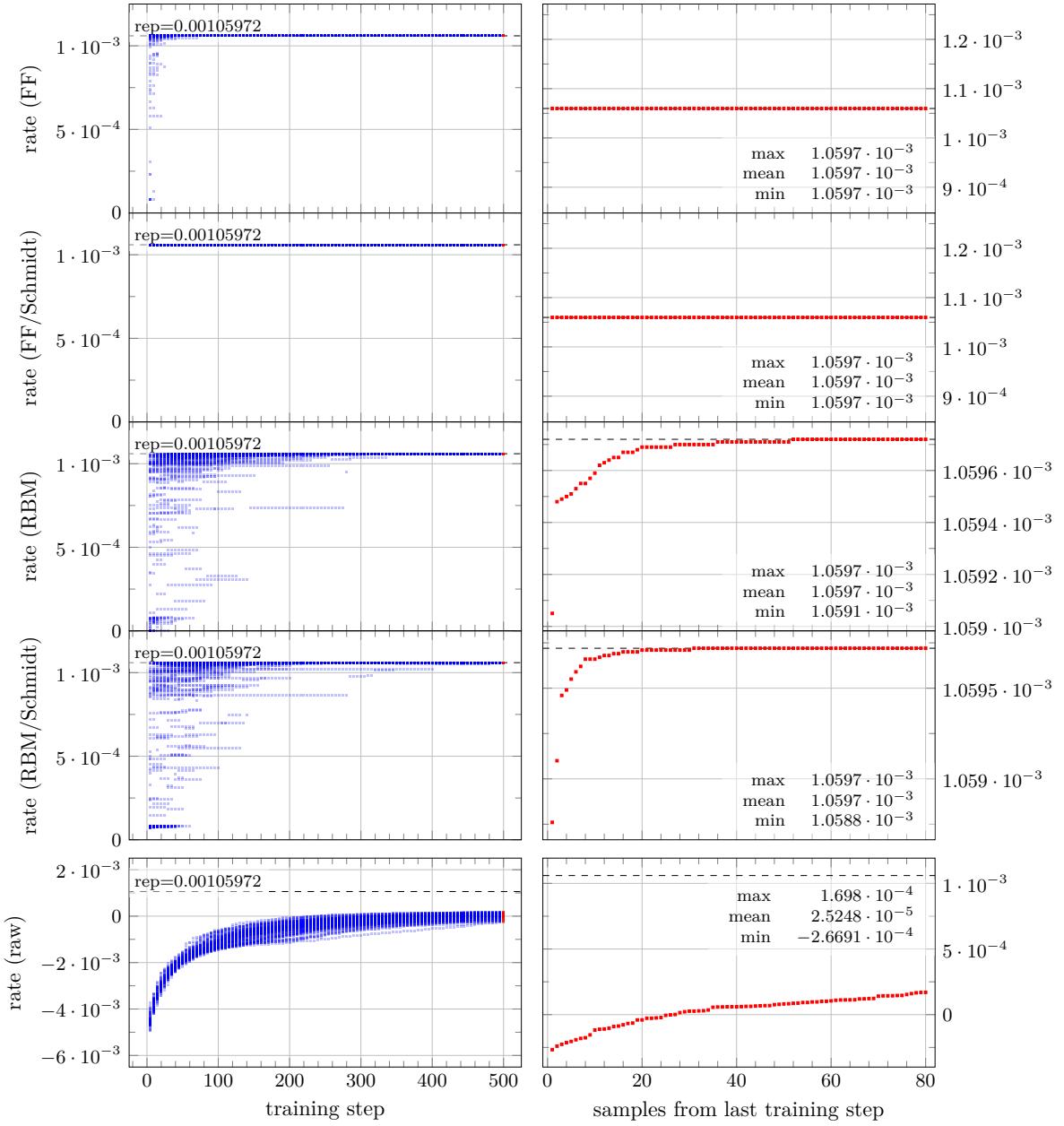


Figure 11: Training convergence of a particle swarm (PSO) algorithm implemented in pagmo, maximizing the CI of three copies of the depolarizing channel  $\mathcal{D}_p$ , with noise parameter  $p = 0.2523$ . The network architectures are identical to the ones in Fig. 2.

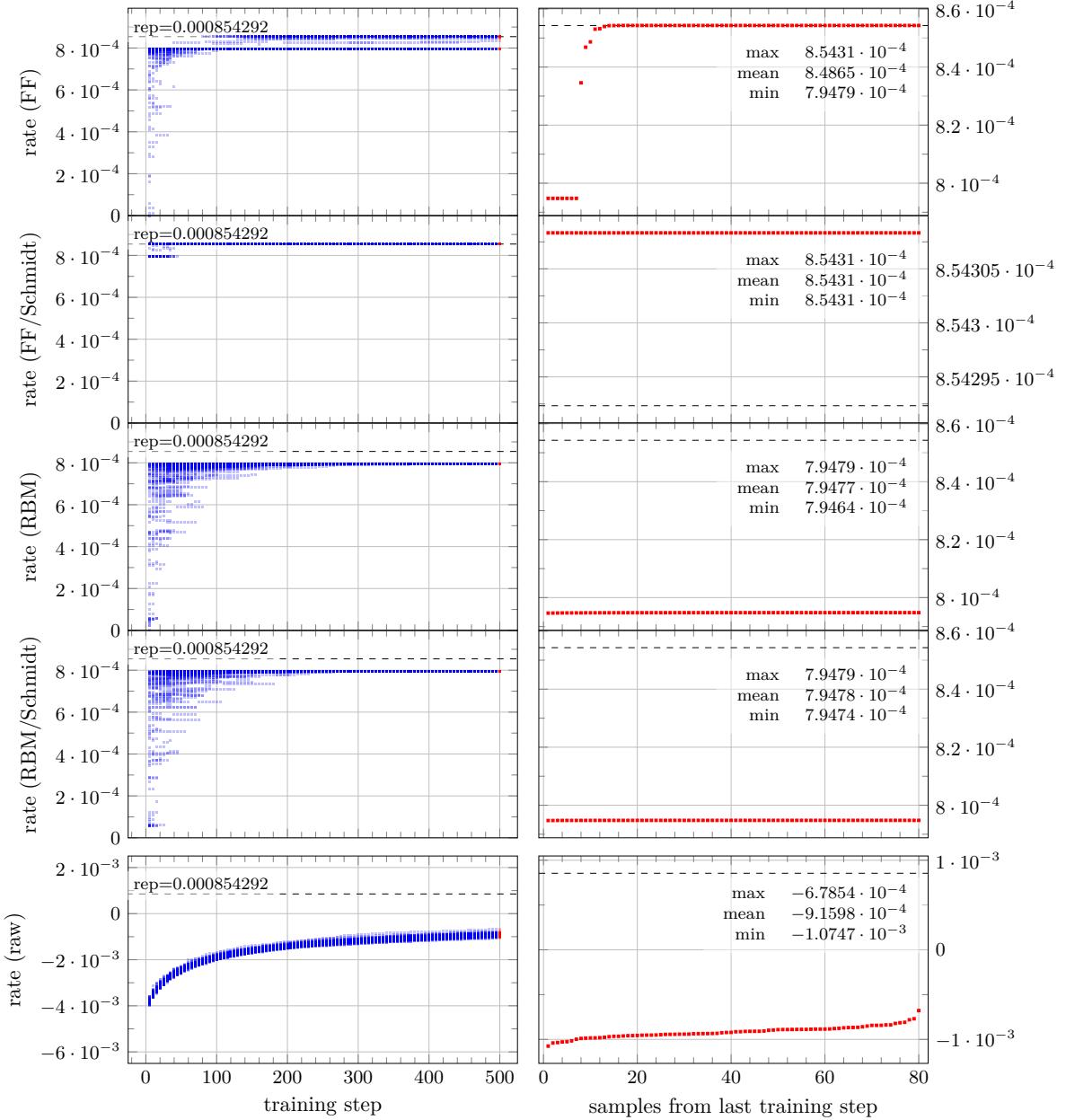


Figure 12: Training convergence of a particle swarm (PSO) algorithm implemented in pagmo, maximizing the CI of four copies of the depolarizing channel  $\mathcal{D}_p$ , with noise parameter  $p = 0.2523$ . The network architectures are identical to the ones in Fig. 2.

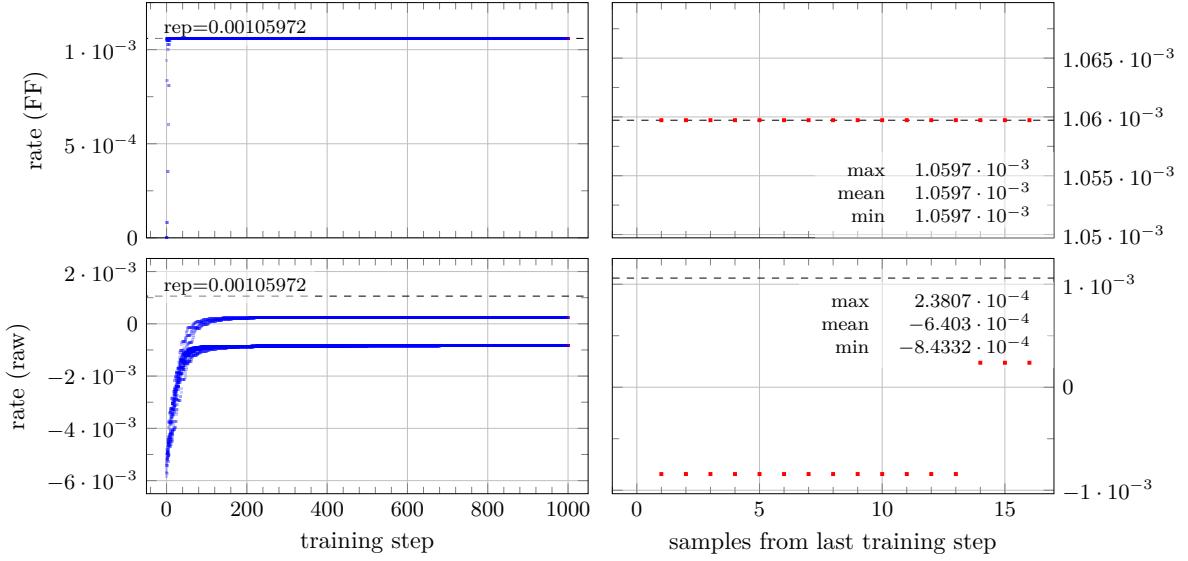


Figure 13: Training convergence of a particle swarm (PSO) algorithm implemented in MATLAB, maximizing the CI of three copies of the depolarizing channel  $\mathcal{D}_p$ , with noise parameter  $p = 0.2523$ . The network architectures are identical to the ones in Fig. 2.

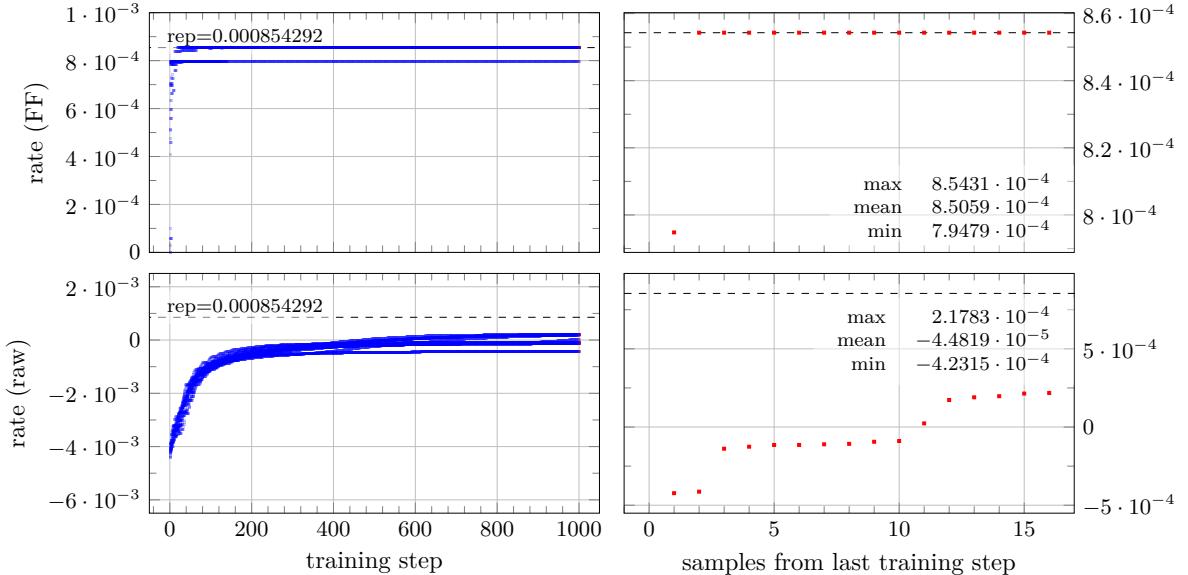


Figure 14: Training convergence of a particle swarm (PSO) algorithm implemented in MATLAB, maximizing the CI of four copies of the depolarizing channel  $\mathcal{D}_p$ , with noise parameter  $p = 0.2523$ . The network architectures are identical to the ones in Fig. 2.

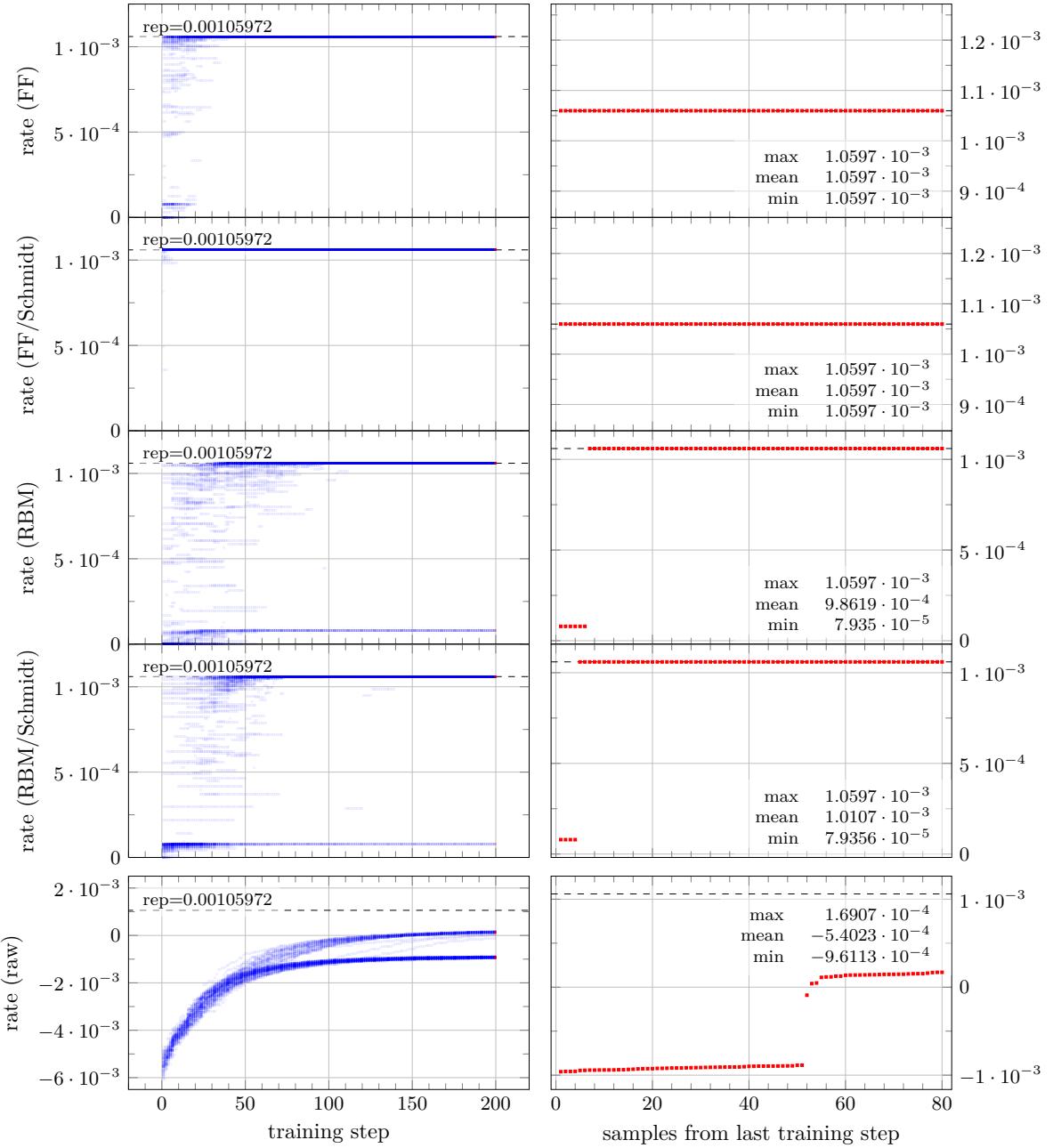


Figure 15: Training convergence of a simple genetic (SGE) algorithm implemented in pagmo, maximizing the CI of three copies of the depolarizing channel  $\mathcal{D}_p$ , with noise parameter  $p = 0.2523$ . The network architectures are identical to the ones in Fig. 2.

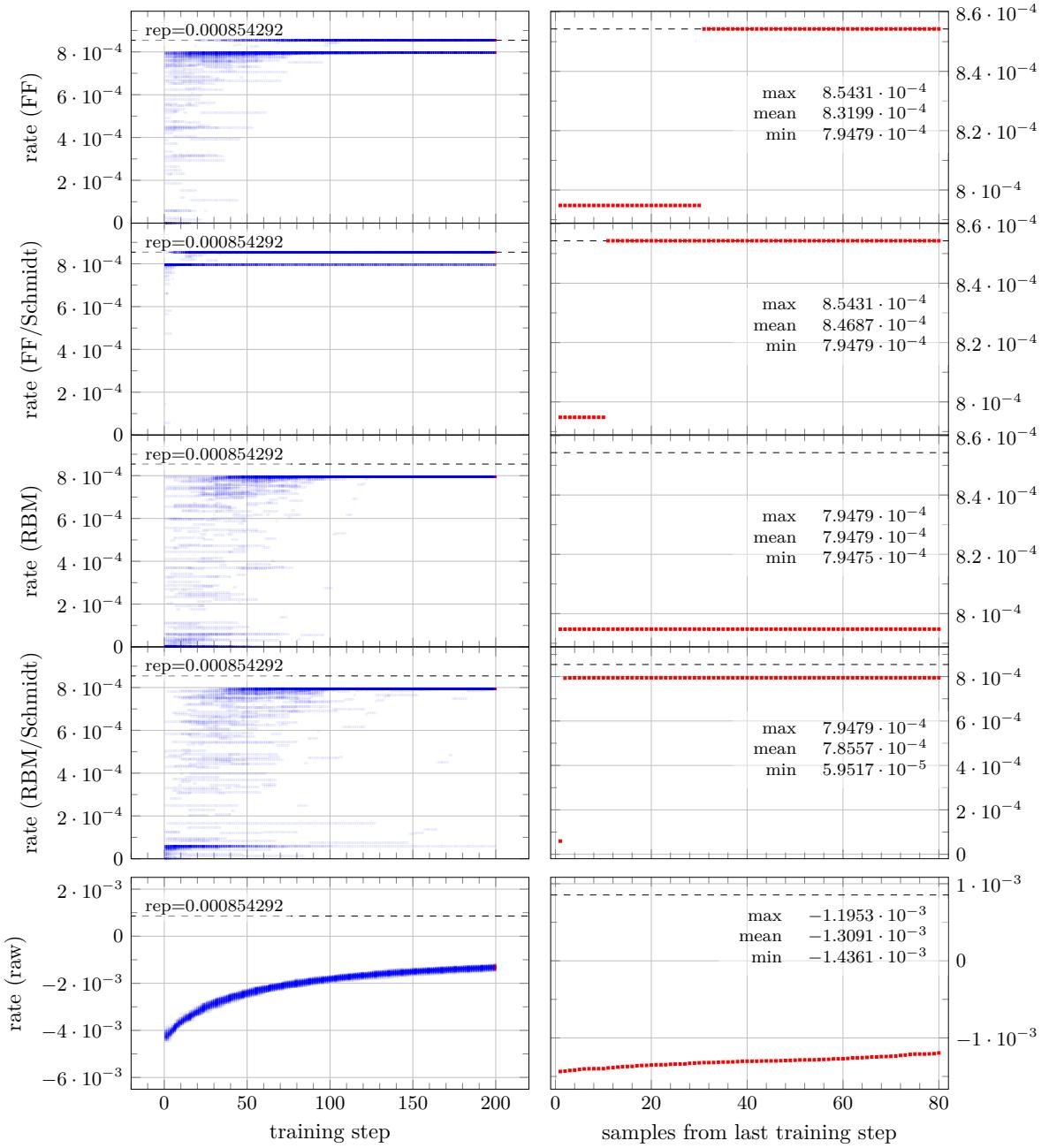


Figure 16: Training convergence of a simple genetic (SGE) algorithm implemented in pagmo, maximizing the CI of four copies of the depolarizing channel  $\mathcal{D}_p$ , with noise parameter  $p = 0.2523$ . The network architectures are identical to the ones in Fig. 2.