Fidelity bounds for storage and retrieval of von Neumann measurements

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This work examines the problem of learning an unknown single-qubit von Neumann measurements from a finite number of copies. To obtain a faithful approximation of the given measurement we are allowed to use it \( N \) times. Our main goal is to estimate an asymptotic behavior of the maximum value of the average fidelity function \( F \) for a general \( N \to 1 \) learning scheme. We obtained results showing that \( 1 - \frac{1}{N} \leq F \leq 1 - \Theta \left( \frac{1}{N^2} \right) \). In addition to that, we discovered a particular class of learning schemes, which we call the pretty good learning scheme. This scheme, despite its lack of optimality, provides a relatively high value for \( F \), asymptotically behaving as \( 1 - \frac{1}{N} \). Additionally, it employs a simple storage strategy, which uses only two-qubit entangled memory states and the learning process is done in parallel. Finally, the fidelity function calculated for the pretty good learning scheme is uniform over all single-qubit von Neumann measurements.

I. INTRODUCTION

Alongside the recent surge in classical machine learning (ML) research, a quantum equivalent of learning has been considered by the scientific community [1][3]. As this research enters the quantum realm, we have a greatly expanded area of possible approaches. Aside from the classical data–classical algorithms approach, we can consider how classical algorithms can enhance quantum computing. One of such examples is the simulation of many-body systems [4].

Another approach to quantum machine learning (QML) focuses on exploiting quantum algorithms yet keeping the input data classical [5][7]. At first glance, the area shows promise of a potential exponential speedup for specific tasks, but there is some contention whether the problem of loading classical data into quantum devices negates all the possible advantages [3].

Finally, we arrive at the setting of interest for this work. In it, both the data and the algorithms are quantum. Roughly speaking, we are interested in the case when we are given access to a black box performing a quantum operation, and our goal is to develop a scheme that will approximate that operation at a later time [9][15].

For someone coming from a classical computing field, this problem might seem a bit artificial, yet in quantum computing, we can not clone arbitrary quantum bits [10]. Going even further, we have what is known as the no-programming theorem [17], which states that general processors, which perform a program based on some input state, are not possible. There is no doubt that programmable devices would represent an instrumental piece of quantum technology. Hence, their approximate realizations are of common interest [18][19]. In the literature, this task is also called storage and retrieval (SAR).

In the general approach of SAR we want to approximate \( k \) times a given, unknown operation, which we were able to perform \( N \) times experimentally. Such scheme is called as \( N \to k \) learning scheme. Our main goal is to find the optimal learning strategy. This strategy usually consists of preparing some initial quantum state, applying the unknown operation \( k \) times, which allows us to store the unknown operation for later use, and finally a retrieval operation that applies an approximation of the black box on some arbitrary quantum state. Additionally, each application of the operation contained within the black box can be followed by some arbitrary processing operations. If that is the case, the optimal strategy should also contain their description. The scheme is optimal when it achieves the highest possible fidelity of the approximation [20][21].

The seminal work in this field was the paper by Bisio and Chiribella [22] devoted to learning an unknown unitary transformation. Therein, the authors focused on storing the unitary operation in a quantum memory while having a limited amount of resources. They proved unitary operations could be learned optimally in the parallel scheme, which means there are no additional processing after the usage of the unknown unitary transformation. Hence, all the required uses of the black box can be performed in parallel. They also provide an upper bound on the fidelity of such a scheme for the case of \( N \to 1 \) learning: \( 1 - \frac{1}{N} \). A probabilistic version of SAR (PSAR) prob-
lem was also considered in \cite{23,24}. There, they showed the optimal success probability of $N \rightarrow 1$ PSAR of unitary channels on $d$-dimensional quantum systems is equal to $N/(N-1+d^2)$.

Subsequent works build upon these results but focus on different classes of operations, for example, the von Neumann measurements \cite{25}. In contrast to previous works, they showed that in general the optimal algorithm for quantum measurement learning cannot be parallel and found the optimal learning algorithm for arbitrary von Neumann measurements for the case $1 \rightarrow 1$ and $2 \rightarrow 1$. Nevertheless, a general optimal scheme $N \rightarrow 1$ of measurement learning still remains an open problem, even for low-dimensional quantum systems. Hence, investigation of SAR for von Neumann measurements, despite some partial results, is still an open question.

In this work, we address the unsolved problem of learning an unknown qubit von Neumann measurement defined in \cite{25}. We focus on fidelity bounds for a general $N \rightarrow 1$ scheme of learning qubit von Neumann measurements. To find the lower bound, we introduce a pretty good learning scheme for which, the value of the average fidelity function behaves as $1 - \frac{1}{N}$. This scheme is a particular case of parallel learning scheme and it uses only two-qubit entangled memory states. The fidelity function calculated for the pretty good learning scheme is uniform over all qubit von Neumann measurements. Moreover, we provide the upper bound for the average fidelity function, which is equal $1 - \Theta \left( \frac{1}{N^2} \right)$. Although both of these bounds differ and leave room for improvement, numerical investigations suggest that the upper bound can be tightened to $1 - \Theta \left( \frac{1}{N} \right)$.

This paper is organized as follows. In Section \ref{II} we formulate the problem of von Neumann measurement learning. In Section \ref{IIA} we introduce necessary mathematical concepts. Our main result is then presented in Sec. \ref{II} (Theorem 1), by first addressing the case of lower bound (Subsection \ref{II.4}), and subsequently upper bound (Subsection \ref{II.3}). Additionally, in this Section we focus on numerical results which additionally conjecture that the upper bound should behave as $1 - \Theta \left( \frac{1}{N} \right)$. Finally, Sec. \ref{IV} concludes the article with a summary of the main results. In Appendix we provide more details of proofs for average fidelity function bounds.

II. PROBLEM FORMULATION

In this section we present the formulation of the problem of learning an unknown von Neumann measurement. We provide an overview of a learning scheme in Fig. 1 along with its description in Subsection \ref{II.3}.

A. Mathematical framework

Let us introduce the following notation. Consider a $d$-dimensional complex Euclidean space $\mathbb{C}^d$ and denote it by $\mathcal{H}_d$. Let $M(\mathcal{H}_{d_1}, \mathcal{H}_{d_2})$ be the set of all matrices of dimension $d_1 \times d_2$. As a shorthand we put $M(\mathcal{H}_d) := M(\mathcal{H}_{d_1}, \mathcal{H}_{d_2})$. The set of quantum states defined on space $\mathcal{H}_d$, that is the set of positive semidefinite operators having unit trace, will be denoted by $\Omega(\mathcal{H}_d)$. We will also need a linear mapping transforming $M(\mathcal{H}_{d_1})$ into $M(\mathcal{H}_{d_2})$ as $T : M(\mathcal{H}_{d_1}) \mapsto M(\mathcal{H}_{d_2})$. There exists a bijection between introduced linear mappings $T$ and set of matrices $M(\mathcal{H}_{d_1,d_2})$, known as the Choi-Jamiołkowski isomorphism \cite{26,27}. Its explicit form is $T = \sum_{i,j=0}^{d_1-1} T(|i\rangle\langle j|) \otimes |i\rangle\langle j|$. We will denote linear mappings with calligraphic font $\mathcal{L}, \mathcal{S}, T$ etc., whereas the corresponding Choi-Jamiołkowski matrices as plain symbols: $L,S,T$ etc. Moreover, we introduce the vectorization operation of a matrix $X \in M(\mathcal{H}_{d_1}, \mathcal{H}_{d_2})$, defined by $|X\rangle := \sum_{i=0}^{d_2-1} (X| i\rangle) \otimes |i\rangle$.

A general quantum measurement (POVM) $\mathcal{Q}$ can be viewed as a set of positive semidefinite operators $\mathcal{Q} = \{Q_i\}_i$ such that $\sum_i Q_i = \mathbf{1}$. These operators are usually called effects. The von Neumann measurements, $\mathcal{P}_U$, are a special subclass of measurements whose all effects are rank-one projections given by $\mathcal{P}_U = \{P_{U,i}\}_{i=0}^{d_2-1} = \{U|i\rangle\langle i|U^\dagger\}_{i=0}^{d_2-1}$ for some unitary matrix $U \in M(\mathcal{H}_d)$.

Quantum channels are completely positive and trace preserving (CPTP) linear maps. Generally, $\mathcal{C}$ is a quantum channel which maps $\mathcal{M}(\mathcal{H}^{(in)})$ to $\mathcal{M}(\mathcal{H}^{(out)})$ if its Choi-Jamiołkowski operator $\mathcal{C}$ is a positive semidefinite and $\text{tr}_{\mathcal{H}^{(out)}}(\mathcal{C}) = \mathbf{1}$, where $\text{tr}_{\mathcal{H}^{(out)}}$ denotes a partial trace over the output system $\mathcal{H}^{(out)}$. Given a von Neumann measurement $\mathcal{P}_U$, it can be seen as a measure-and-prepare quantum channel $\mathcal{P}_U(\rho) = \sum_i \text{tr}\{P_{U,i}\rho\}|i\rangle\langle i|$, $\rho \in \Omega(\mathcal{H}_d)$. The Choi matrix of $\mathcal{P}_U$ is $\Phi_U = \sum_i |i\rangle\langle i| \otimes P_{U,i}$, which will be utilized throughout this work. Finally, we will use the notation $\Phi_U$ to indicate unitary channel given by $\Phi_U(X) = UXU^\dagger$ and the shortcut $\mathcal{I}_d := \Phi_1$ for the identity channel.

B. Learning setup

Figure 1: Schematic representations of the setup for learning of von Neumann measurements $\mathcal{P}_U$ in the $N \rightarrow 1$ scheme.
Imagine we are given a black box, with the promise that it contains some von Neumann measurement, $P_U$, which is parameterized by a unitary matrix $U$. The exact value of $U$ is unknown to us. We are allowed to use the black box $N$ times. Our goal is to prepare some initial memory state $\sigma$, some intermediate processing channels $C_1, \ldots, C_{N-1}$ and a measurement $\mathcal{R}$ such that we are able to approximate $P_U$ on an arbitrary state $\rho$. This approximation will be denoted throughout this work as $Q_U$. We would like to point out that, generally, $Q_U$ will not be a von Neumann measurement.

The initial memory state $\sigma$ and entire sequence of processing channels $\{C_i\}$ can be viewed as storing the unknown operation and will be denoted as $S$ whereas the measurement $\mathcal{R}$ we will call as retrieval. During the storing stage, we apply $S$ on $N$ copies of $P_U$. As a result, the initial memory state $\sigma$ is transferred to the memory state $\sigma_{P_U,S}$. After that, we measure an arbitrary quantum state $\rho$ and the memory state $\sigma_{P_U,S}$ by using $\mathcal{R}$. Equivalently, we can say that during retrieval stage, we apply the measurement $Q_U$ on the state $\rho$. The entire learning scheme will be denoted by $L$ and considered as a triple $L = (\sigma, \{C_i\}_{i=1}^{N-1}, \mathcal{R})$. We emphasize that the procedure allows us to use as much quantum memory as necessary.

As a measure of quality of approximating a von Neumann measurement $P_U = \{P_{U,i}\}_i$ with a POVM $Q_U = \{Q_{U,i}\}_i$, we choose the fidelity function $\mathcal{F}$, which is defined as follows

$$\mathcal{F}(P_U, Q_U) := \frac{1}{d} \sum_i \text{tr}(P_{U,i} Q_{U,i}),$$

where $d$ is the dimension of the measured system. Note that in the case when $P_U$ is a von Neumann measurement we obtain the value of fidelity function $\mathcal{F}$ belongs to the interval $[0, 1]$ and equals to one if and only if $P_{U,i} = Q_{U,i}$ for all $i$. As there is no prior information about $P_U$ provided, we assume that $U$ is sampled from a distribution pertaining to the Haar measure. Therefore, considering a von Neumann measurement $P_U$ and its approximation $Q_U$ we introduce the average fidelity function $\mathcal{F}_{avg}$ with respect to Haar measure as

$$\mathcal{F}_{avg} := \int_U dU \mathcal{F}(P_U, Q_U).$$

Our main goal is to maximize $\mathcal{F}_{avg}$ over all possible learning schemes $L = (\sigma, \{C_i\}_{i=1}^{N-1}, \mathcal{R})$. We introduce the notation of the maximum value of the average fidelity function

$$F := \max_L \mathcal{F}_{avg},$$

III. FIDELITY BOUNDS

In this section we present our main results – the lower and upper bounds for the average fidelity function $F$ for learning of single-qubit von Neumann measurements. We will provide sketches of proofs and a general intuition behind our results. The full proofs are postponed to the Appendix, due to their technical nature. All the discussion presented in this section can be summarized as the following theorem.

**Theorem 1.** Let $F$ be the maximum value of the average fidelity function, defined in Eq. (3) for the $N \rightarrow 1$ learning scheme of single-qubit von Neumann measurements. Then, $F$ can be bounded as

$$1-\frac{1}{N} \leq F \leq 1 - \Theta\left(\frac{1}{N^2}\right).$$

A. Lower bound

The proof of the lower bound for $F$ is constructive, by which we mean that we will construct the learning scheme of single-qubit von Neumann measurements, which achieves this bound. This scheme will be called the pretty good learning scheme. Let us consider a parallel learning scheme $\mathcal{P}_U$ with $N$ copies of the von Neumann measurement $P_U$. A sketch of our scheme is shown in Fig. 2 and here we present the algorithm describing the procedure:

1. We prepare the initial memory state $\sigma$ as a tensor product of $N$ maximally entangled states $\omega := \frac{1}{\sqrt{2}} \langle 1_2 |$.

![Figure 2: Schematic representations of the pretty good learning scheme for $N = 3$. In the learning process we obtained three labels: 0, 1, 0. As labels “0” are in majority, we reject the label “1” and the associated quantum part.](image)
2. We partially measure each state $|\omega\rangle$ using $\mathcal{P}_U$, obtaining the state $\langle \mathcal{P}_U \otimes I_2 | \omega \rangle \langle \omega | \mathcal{P}_U \rangle$.

3. For each measurement $\mathcal{P}_U$, we obtain one of two possible measurement results: “0” or “1”. In consequence, we get $N_0$ outcomes “0” and $N_1$ outcomes “1”, $N_0 + N_1 = N$. The state of the remaining quantum part is equal to $\mathcal{P}_{U,0} \otimes \mathcal{P}_{U,1}$ (up to permutation of subsystems). Without loss of a generality (w.l.o.g.), we may assume that $N_0 \geq N_1$.

4. By majority vote we reject minority report, i.e. we reject all outcomes “1” and quantum states associated with them. As a result the memory state is given by $\sigma_{\mathcal{P}_U, S} = \mathcal{P}_{U,0} \otimes \mathcal{P}_{U,0}$.

5. We prepare an arbitrary state $\rho \in \Omega(\mathcal{H}_2)$.

6. We perform a binary retrieval measurement $\mathcal{R} = \{R, \mathbb{1} - R\}$ on $\rho \otimes \sigma_{\mathcal{P}_U, S}$.

To construct the effect $R$, let us fix $N_0$ and let $n = N_0 - 1$. We introduce the family of Dicke states $|D_k^n\rangle$. The Dicke state $|D_k^n\rangle$ is the $n$-qubit state, which is equal to the superposition state of all $\binom{n}{k}$ basis states of weight $k$. For example, $|D_1^2\rangle = \frac{1}{\sqrt{3}} (|00\rangle + |01\rangle + |10\rangle)$. Let us also define

$$s_n(k, m) := \sum_{i+j=m} \delta_{i+j=m} \binom{k}{i} \binom{n-k}{j} (-1)^{n-k-j}$$

being the convolution of binomial coefficients. Consider the effect $R$ of the form

$$R = \sum_{k=0}^{n} |R_k\rangle \langle R_k|,$$  

where $|R_k\rangle := \frac{|M_k\rangle}{\|M_k\|}$ and matrices $M_k \in M(\mathcal{H}_2, \mathcal{H}_{2^{m+1}})$ are given by

$$M_k = \sum_{m=0}^{n+1} \frac{s_n(k, n-m)|0\rangle + s_n(k, n+1-m)|1\rangle}{\sqrt{\binom{n+1}{m}}} \langle D_m^{n+1} |$$

for $k = 0, \ldots, n$. The proof that $R$ is a valid effect is relegated to Lemma 5 in Appendix A. In this learning scheme the approximation $Q_U = \{Q_{U,0}, Q_{U,1} - Q_{U,0}\}$ is determined by relation $\text{tr} (\rho Q_{U,0}) = \text{tr} \left( \left( \rho \otimes \mathcal{P}_{U,0} \otimes \mathcal{P}_{U,0} \right) R \right)$. Basing on Lemma 6 in Appendix A, the effect $Q_{U,0}$ has the form

$$Q_{U,0} = \frac{N_0}{N_0 + 1} \mathcal{P}_{U,0}.$$  

Provided we observed $N_0$ outcomes “0”, we have that $\mathcal{F}(\mathcal{P}_U, Q_U) = \frac{2N_0 + 1}{2N_0 + 2}$, where $N_0$ satisfies $N_0 \geq \lceil \frac{N}{2} \rceil$. Note, that the value of $\mathcal{F}(\mathcal{P}_U, Q_U)$ does not depend on the choice of $U$. The average fidelity function $\mathcal{F}_{\text{avg}}$ defined for the pretty good learning scheme of qubit von Neumann measurements satisfies

$$\mathcal{F}_{\text{avg}} = \frac{2N_0 + 1}{2N_0 + 2} \geq \frac{2\left\lceil \frac{N}{2} \right\rceil + 1}{2\left\lceil \frac{N}{2} \right\rceil + 2}. \quad (9)$$

Therefore, we conclude that our construction gives the following lower bound for $F$ defined in Eq. (3)

$$F \geq \frac{2\left\lceil \frac{N}{2} \right\rceil + 1}{2\left\lceil \frac{N}{2} \right\rceil + 2} \geq 1 - \frac{1}{N}, \quad (10)$$

which finishes the first part of the proof.

**Corollary 1.** In the pretty good learning scheme $\mathcal{L}_{\text{PGLS}} = (\sigma, \{C_i\}_{i=1}^{N-1}, R)$ the initial state $\sigma$ is defined as a product of $N$ copies of maximally entangled state $|\omega\rangle$, processing channels $\{C_i\}_{i=1}^{N-1}$ are responsible for majority voting and the measurement $\mathcal{R} = \{R, \mathbb{1} - R\}$ is defined by Eq. (6).

Finally, averaging the construction of $Q_U$ over all possible combinations of measurements’ results $\{0, 1\}^N$ leads to the following approximation of $\mathcal{P}_U$.

**Corollary 2.** The approximation $Q_U$ is a convex combination of the original measurement $\mathcal{P}_U$ and the maximally depolarizing channel $\Phi_\ast$. More precisely,

$$Q_U = \frac{\left\lceil \frac{N}{2} \right\rceil}{\left\lceil \frac{N}{2} \right\rceil + 1} \mathcal{P}_U + \frac{1}{\left\lceil \frac{N}{2} \right\rceil + 1} \Phi_\ast. \quad (11)$$

**B. Upper bound**

In order to show the upper bound for $F$, we will construct a different learning scheme based on learning of unitary maps. It will provide us the desired inequality. Next, we will discuss the tightness on this inequality, and show evidences suggesting that asymptotically, the pretty good learning scheme is “near optimal” (in the asymptotic notation).

**Lemma 1.** The maximum value of the average fidelity function, defined in Eq. (3) is upper bounded by

$$F \leq 1 - \Theta \left( \frac{1}{N^2} \right). \quad (12)$$

The complete proof of Lemma 1 is shown in Appendix B. As in the previous section, here we will only sketch the key steps.

Let us consider a new learning scheme presented in Fig. 3. In this scheme, we are given $N$ copies of unitary channel $\Phi_U$, which we can use in parallel. We want to approximate the measurement $\mathcal{P}_U$, but using the black
Figure 3: Schematic representation of the setup, which we use to upper bound $F$. In this scenario, we are given $N$ copies of unitary channel $\Phi_U$ in parallel. Our objective is to approximate the von Neumann measurement $P_U.$

box with the unitary channel $\Phi_U$ inside. We will choose appropriate initial memory state $|\psi\rangle$ and retrieve binary measurement $\mathcal{R} = \{R_0, R_1\}$. We use the same measures of quality of approximating the measurement $P_U$ with $Q_U$ as before, namely $F$ defined in Eq. (1) and $\mathcal{F}_{\text{avg}}$ defined in Eq. (2). The goal is then, to maximize the value of the average fidelity function, which in this case, we will denote as $F_p$. In the Appendix B1 we derived the formula for $F_p$, which is given by

$$F_p = \max_{\mathcal{R}, |\psi\rangle} \int dU \sum_{i=0}^{1} \text{tr} \left[ R_i \left( P_{U,i} \otimes (\Phi_U \otimes I) \langle \psi | \psi \rangle \right) \right].$$

(13)

Calculating the value of $F_p$ is the crux of the proof, because we managed to show that $F \leq F_p$ (see Lemma 1 in Appendix B3). We derived the thesis of Lemma 1 by achieving the inequality $F_p \leq 1 - \Theta \left( \frac{1}{\sqrt{N}} \right).$

**Corollary 3.** There is no perfect learning scheme for von Neumann measurements, i.e., for any $N \in \mathbb{N}$ the value of $F$ is always smaller than 1.

Below we discuss the tightness of $F_p \leq 1 - \Theta \left( \frac{1}{\sqrt{N}} \right)$ and present some numerical and analytical considerations which suggest, that the upper bound can be tightened to $1 - \Theta \left( \frac{1}{N} \right)$.

**Conjecture 1.** The maximum value of the average fidelity function $F_p$, defined in Eq. (13) is not greater than $\frac{2N+1}{2N+2}$.

The above conjecture is supported by the following evidences. First, in Proposition 1 in Appendix B3 we proved that for any $N \in \mathbb{N}$ and for fixed memory state $|\psi\rangle$ of the form $|\psi\rangle = |0\rangle^\otimes N$ we get $F_p \leq \frac{2N+1}{2N+2}$. In particular, based on the proof in Appendix B3 we concluded, that for $N = 1$ the conjecture is fulfilled. Moreover, in Proposition 2 in Appendix B3 we showed that the conjecture is also true for $N = 2$ for the choice of the state $|\psi\rangle = |0\rangle |0\rangle$. What is more, our numerical investigation, which we run for $N = 3, 4, 5$, confirms that the conjecture also holds in these cases. In the numerical analysis, we used the fact that Eq. (13) can be expressed as the probability of correct discrimination of channels $\Psi_i(X) = \int dU (U \otimes U^\otimes N) \langle i | i \rangle X (U^\dagger \otimes U^\dagger)^\otimes N$ with the assistance of entanglement. Due to the Holevo-Helstrom results [30] the upper bound of $F_p$ can be directly calculated via the diamond norm [30] in the following way $F_p \leq \frac{1}{2} + \frac{1}{2} \| \Psi_0 - \Psi_1 \|_d$. To optimize this problem we used the Julia programming language along with package QuantumInformation.jl [31]. The code is available on GitHub [32].

Finally, we want to add that $F_p \geq \frac{2N+1}{2N+2}$, which strengthen out conjecture. To obtain a such result we take $|\psi\rangle = |0\rangle^\otimes N$ and $\mathcal{R} = \{R, 1 - R\}$ defined by Eq. (9) for $N_0 = N$.

**IV. CONCLUSIONS AND DISCUSSION**

In this work, we studied the problem of learning of $N$ copies of qubit von Neumann measurements. Our goal was to find bounds for the maximum value of the average fidelity function $F$. It was considered over all possible learning schemes, and the average was taken over all von Neumann measurements. The search for the bounds led us to a special class of learning schemes, which we dubbed the pretty good learning scheme. Despite its lack of optimality it provides relatively high value for the average fidelity function, which asymptotically behaves as $1 - \frac{1}{N}$. The proposed learning scheme is a variation of the parallel one and employs a simple storage strategy. Moreover, it turned out that achieved the value of fidelity function is uniform over all von Neumann measurements. It also provides a non-trivial lower bound of the form $F \geq 1 - \frac{1}{N}$.

In addition to that, we provided the upper bound for $F$, which asymptotically behaves as $F \leq 1 - \Theta \left( \frac{1}{\sqrt{N}} \right)$. Especially, it implies it is not possible to approximate perfectly von Neumann measurement $P_U$ in $N \rightarrow 1$ learning scheme for any $N \in \mathbb{N}$. Based on the numerical investigation, we discuss the tightness of this bound. With additional analytical results we conjecture that the upper bound should also behave as $1 - \Theta \left( \frac{1}{N} \right)$, which remains an open question.

This work paves the way towards a full description of capabilities of von Neumann measurement learning schemes. One potential way forward is the probabilistic storage and retrieval approach, widely studied for unitary operations and phase rotations in [23, 24]. According to our numerical results, the probability of retrieval of a quantum measurement in a parallel scheme is exactly $N/(N + 3)$, which corresponds to the value obtained in [23] for unitary channels, while adaptive strategies for quantum measurements learning provide slightly higher probability, starting from $N \geq 3$. 
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Permanent link to code/repository, Accessed: 2022-03-28.
Appendix A: Proof of lower bound

The pretty good learning scheme $L_{\text{PGLS}} = (\sigma, \{C_i\}_{i=1}^{N-1}, R)$ consists of the initial state $\sigma$, which is a tensor product of $N$ copies of the maximally entangled state $|\omega\rangle = \frac{1}{\sqrt{N}} |\mathbb{I}_2\rangle$, processing channels $\{C_i\}_{i=1}^{N-1}$ that are responsible for majority voting (see Section IIIA) and the measurement $R = \{R, \mathbb{1} - R\}$. To construct the effect $R$, we fix $N_0 \in \mathbb{N}$ and take $n = N_0 - 1$. Let us define

$$s_n(k, m) := \sum_{i=0}^{k} \sum_{j=0}^{n-k} \delta_{i+j-m} \binom{k}{i} \binom{n-k}{j} (-1)^{n-k-j},$$

being the convolution of binomial coefficients. We consider the effect $R$ of the form

$$R = \sum_{k=0}^{n} |R_k\rangle\langle R_k|, \quad \text{such that } |R_k\rangle = \frac{|M_k\rangle}{||M_k||_2},$$

$$M(\mathcal{H}_2, \mathcal{H}_{2^{n+1}}) \ni M_k = \sum_{m=0}^{n+1} s_n(k, n-m) |0\rangle + s_n(k, n+1-m) |1\rangle \langle D^m |,$$

for $k = 0, \ldots, n$. To prove the lower bound for $F$ we introduce the following lemmas.

**Lemma 2.** Let $|x\rangle = \begin{bmatrix} a \\ b \end{bmatrix}, a, b \in \mathbb{C}$. Then, we have $M_k |x\rangle^{\otimes n+1} = (a + b)^k (a - b)^{n-k} |x\rangle$.

**Proof.** Direct calculations reveal

$$M_k |x\rangle^{\otimes n+1} = \left[ \sum_{m=0}^{n+1} \binom{n+1}{n-m} s_n(k, m) a^m b^{n-m} \right] = \sum_{m=0}^{n+1} s_n(k, m) a^m b^{n-m} |x\rangle = (a + b)^k (a - b)^{n-k} |x\rangle.$$  \hfill (A3)

To prove that $R$ is a valid effect, let us now define

$$M := [s_n(k, m)]_{k,m=0}^{n},$$

and a diagonal matrix

$$D := \sum_{m=0}^{n+1} \frac{1}{\binom{n+1}{m}} |m\rangle\langle m|.$$  \hfill (A5)

**Lemma 3.** With the notation given above, it holds that $M^2 = 2^n \mathbb{1}_{n+1}$.

**Proof.** First, observe that $\mathbb{C}^{n+1} = \text{span}( |x\rangle)_{k=0}^{n} : x \in \mathbb{C}$, where $x \in \mathbb{C}$. We have

$$M |x\rangle = \left[ \sum_{m=0}^{n} s_n(k, m) a^m \right]_{k=0}^{n} = \left[ (x+1)^k (x-1)^{n-k} \right]_{k=0}^{n} = \left[ \frac{x+1}{x-1} \right]_{k=0}^{n} = (x-1)^n \left[ \frac{x+1}{x-1} \right]_{k=0}^{n}. \hfill (A6)$$

Finally, we calculate

$$M^2 |x\rangle = (x-1)^n \left( \frac{x+1}{x-1} \right)^n \left[ \frac{x+1}{x-1} \right]_{k=0}^{n} = 2^n |x\rangle.$$  \hfill (A7)

**Lemma 4.** Using the notation presented above, we have the following equation $MD = (MD)^\top$. 

---

\[ \sum_{i=0}^{k} \sum_{j=0}^{n-k} \delta_{i+j-m} \binom{k}{i} \binom{n-k}{j} (-1)^{n-k-j}, \]
Proof. We will show that \( \langle k | MD | m \rangle = \langle m | MD | k \rangle \) for any \( m, k = 0, \ldots, n \). W.l.o.g. we can assume that \( k < m \). On the one hand, it holds that

\[
\langle k | MD | m \rangle = \sum_{j=0}^{n} \frac{(-1)^{n-j} \binom{k}{j} \binom{n-j}{k}}{\binom{n}{m}}
\]

\[
= \sum_{i=\max(0, m+k-n)}^{k} \frac{(-1)^{k-m+i} \binom{m}{i} \binom{n-m}{k-i}}{\binom{n}{m}}
\]

(A8)

On the other hand, we can calculate

\[
\langle m | MD | k \rangle = \sum_{j=0}^{n} \frac{(-1)^{n-j} \binom{m}{j} \binom{n-j}{m}}{\binom{n}{k}}
\]

\[
= \sum_{i=\max(0, m+k-n)}^{k} \frac{(-1)^{k-m+i} \binom{m}{i} \binom{n-m}{k-i}}{\binom{n}{k}}
\]

(A9)

which gives us the desired equality and completes the proof.

Lemma 5. The operator \( R \) defined in Eq. (A2) satisfies \( 0 \leq R \leq \mathbb{I}_{2^{n+2}} \) and therefore \( R = \{R, 1 - R\} \) is a valid POVM.

Proof. Let us fix \( N_0 \in \mathbb{N} \) and take \( n = N_0 - 1 \). Let us consider a matrix \( X := \frac{n+2}{n+1} MDM^\top \). On the one hand, by using Lemma 3 and Lemma 4, we get

\[
X = \frac{n+2}{n+1} (MD)^\top M^\top = \frac{n+2}{n+1} D(M^2)^\top = \frac{n+2}{n+1} 2^n D.
\]

(A10)

On the other hand, we have

\[
\text{tr} \left( M_k^\dagger M_{k'} \right) = \sum_{m=0}^{n} \frac{s_n(k, m)s_n(k', m)}{\binom{n+1}{m}^2} \sum_{m=0}^{n} \frac{s_n(k, m)s_n(k', m)}{\binom{n+1}{m}^2} = \sum_{m=0}^{n} \frac{s_n(k, m)s_n(k', m)}{\binom{n+1}{m}^2} \left[ \frac{1}{n-m} + \frac{1}{n-m+1} \right]
\]

\[
= \frac{n+2}{n+1} \sum_{m=0}^{n} \frac{s_n(k, m)s_n(k', m)}{\binom{n}{m}} = \langle k | X | k' \rangle.
\]

(A11)

Therefore, for all \( k \neq k' \) we get \( \text{tr} \left( M_k^\dagger M_{k'} \right) = 0 \). According to the definition Eq. (A2), we get \( \langle R_k | R_{k'} \rangle = \delta_{k,k'} \), which gives us \( 0 \leq R \leq \mathbb{I}_{2^{n+2}} \).

Lemma 6. Let us fix \( N_0 \in \mathbb{N} \). The approximation \( Q_U = \{Q_{U,0}, \mathbb{I}_2 - Q_{U,0}\} \) of the von Neumann measurement \( \mathcal{P}_U \) obtained in the pretty good learning scheme is of the form

\[
Q_{U,0} = \frac{N_0}{N_0 + 1} P_{U,0}.
\]

(A12)

Proof. Given a unitary matrix \( U \) we take \( P_{U,0} = |x\rangle \langle x| \) for some unit vector \( |x\rangle \in \mathcal{H}_2 \). Let us decompose the \((n+2)\)-qubit space in the following way \( \mathcal{H}_{2^{n+2}} = Z \otimes \mathcal{X} \), where \( Z = \mathcal{H}_2 \) and \( \mathcal{X} = \mathcal{H}_{2^{n+1}} \). In the proof of Lemma 5 we defined the matrix \( X = \frac{n+2}{n+1} MDM^\top \) and showed that \( X = \frac{n+2}{n+1} 2^n D \), and \( \text{tr} \left( M_k^\dagger M_{k'} \right) = \langle k | X | k' \rangle \). Therefore, for
any $k = 0, \ldots, n$ we have $\|M_k\|_2^2 = \frac{n+2}{n+1} 2^n$. Due to this fact and by Lemma 2 we may express the effect $Q_{U,0}$ as

$$Q_{U,0} = \text{tr}_\chi \left( \left( 1_2 \otimes R_{U,0}^{\otimes n+1} \right) R \right) = \left( 1_2 \otimes (x)^{\otimes n+1} \right) R \left( 1_2 \otimes (x)^{\otimes n+1} \right) = \sum_{k=0}^{n} \frac{1}{\|M_k\|_2^2} M_k |x\rangle\langle x|^{\otimes n+1} M_k^\dagger$$

$$= \frac{n+1}{n+2} \sum_{k=0}^{n} 2^n |a+b|^2 |a-b|^{2(n-k)} |x\rangle\langle x|,$$

which completes the proof.

**Appendix B: Proof of upper bound**

In this Appendix we will prove Lemma 1. As a byproduct, we also present some analytical results which support Conjecture 1.

![Figure 4: The schematic representation of a learning scheme $L = (\sigma, \{C_i\}_{i=1}^{N-1}, R)$.](image)

Let us fix $N \in \mathbb{N}$. In the $N \to 1$ learning scheme of single-qubit von Neumann measurements we have access to $N$ copies of a given measurement $P_U$, which is parameterized by some unitary matrix $U \in M(\mathcal{H}_2)$. Let us consider a general single-qubit von Neumann measurement learning scheme $L$, which is depicted in Fig. 4. The Choi-Jamiołkowski representation of $L$ is given as $L = \sum_{i=0}^{1} |i\rangle\langle i| \otimes L_i$, where $|i\rangle \in \mathcal{H}_2^{(\text{out})}$. The result of composition of all copies of $P_U$ and the scheme $L$ is a measurement $Q_U = \{Q_{U,0}, Q_{U,1}\}$, which is an approximation of $P_U$. To define the effects $Q_{U,i}$ we use the link product [28] and $\text{tr}(\rho Q_{U,i}) = \text{tr}(L_i^\dagger (\rho \otimes P_U^{\otimes N}))$ for $\rho \in \Omega(\mathcal{H}_2)$ and $i = 0, 1$. Thus, we can calculate the fidelity defined in Eq. 1 between $P_U$ and $Q_U$

$$F(P_U, Q_U) = \frac{1}{2} \sum_{i=0}^{1} \text{tr}(P_{U,i} Q_{U,i}) = \frac{1}{2} \sum_{i=0}^{1} \text{tr} \left[ L_i^\dagger \left( P_{U,i} \otimes P_U^{\otimes N} \right) \right].$$

Finally, we can express the maximum value of the average fidelity function $F$ defined in Eq. 3 as

$$F = \max_{L} \int_U dU \frac{1}{2} \sum_{i=0}^{1} \text{tr} \left[ L_i^\dagger \left( P_{U,i} \otimes P_U^{\otimes N} \right) \right].$$

In the following subsections we will upper bound $F$ by using thus simplified maximization formula.

1. Measurement learning via parallel storage of unitary transformations

In this section we consider a new learning scheme, presented in Fig. 5. In this scheme, we are given $N$ copies of unitary channel $\Phi_U$, which we can use in parallel. We want to approximate the measurement $P_U$, but using the black box with the unitary channel $\Phi_U$ inside. To do so, we choose an initial memory state $|\psi\rangle \in \mathcal{X} \otimes \mathcal{Y}$ and a retrieval binary measurement $R = \{R_0, R_1\}$, such that $R_i \in M(\mathcal{Z} \otimes \mathcal{X} \otimes \mathcal{Y})$, where $\mathcal{Z} = \mathcal{H}_2^{(n)}$, $\mathcal{X} = \mathcal{H}_{2^N}$ and $\mathcal{Y} = \mathcal{H}_{2^N}$. We want to maximize the value of the average fidelity function, which in this case we will denote as $F_p$. To calculate $F_p$ we may observe that for a given $\rho \in \Omega(\mathcal{Z})$, the probability that outcome $i$ occurs is
Proof. First, we observe that each von Neumann measurement \( \Delta \) is a dephasing channel, given by \( \Delta(X) = \sum_{i=0}^{1} \langle i | X | i \rangle | i \rangle \langle i | \), and a unitary channel \( \Phi_{U,i} \). Equivalently, that means \( \mathcal{P}_U = (\Delta \otimes \mathcal{I}_2)(\langle U \rangle) \). As the channel \( \Delta \) is self-adjoint we obtain
\[
\text{tr} \left[ L_i^T \left( \mathcal{P}_{U,i} \otimes \mathcal{P}_{U}^\otimes \right) \right] = \text{tr} \left[ \left( \mathcal{J}_2 \otimes (\Delta \otimes \mathcal{I}_2) \otimes \mathcal{I}_N \right)(L_i) \right] \tag{B4}
\]
Note that \( \sum_{i=0}^{1} |i \rangle \langle i | \otimes (\Delta \otimes \mathcal{I}_2) \otimes \mathcal{I}_N(L_i) \) represents the composition of the scheme \( \mathcal{L} \) and \( N \) channels \( \Delta \). If we omit processing channels \( \Delta \), we get the following upper bound on \( F \) defined in Eq. \( \text{(B2)} \)
\[
F \leq \max_{\mathcal{L}} \int dU \frac{1}{2} \sum_{i=0}^{1} \text{tr} \left[ L_i^T \left( \mathcal{P}_{U,i} \otimes \mathcal{I}_N \right) \right] = \frac{1}{2} \max_{\mathcal{L}} \int dU \text{tr} \left[ L^T \left( \mathcal{J}_2 \otimes \mathcal{I}_N \right)(\mathcal{J}_2 \otimes U) / (\mathcal{J}_2 \otimes U) \right] \tag{B5}
\]
where \( \mathcal{J}_\Delta \) is Choi-Jamiołkowski representation of \( \Delta \). Observe that the maximal value of the integral in above equation is achievable by networks \( \mathcal{L} \) which satisfy the following commutation relation
\[
[L, \mathbb{I}_2 \otimes U \otimes (\mathbb{I}_2 \otimes U)^\otimes] = 0, \tag{B6}
\]
for any unitary matrix \( U \). To argue this fact, for any \( \mathcal{L} \) one can define a learning network \( \tilde{\mathcal{L}} \) given by
\[
\tilde{\mathcal{L}} = \int dU \left( \mathcal{J}_2 \otimes \mathcal{I}_N \right)(\mathcal{J}_2 \otimes U) / (\mathcal{J}_2 \otimes U) \mathcal{L} \left( \mathcal{J}_2 \otimes U^\dagger \otimes (\mathbb{I}_2 \otimes U)^\otimes \right) \tag{B7}
\]
It is not difficult to show that \( \tilde{\mathcal{L}} \) is a properly defined Choi-Jamiołkowski representation of a quantum learning network [28] Theorem 2.5], which satisfies the relation Eq. \( \text{(B6)} \). Moreover, for both \( \mathcal{L} \) and \( \tilde{\mathcal{L}} \) the value of the integral in Eq. \( \text{(B5)} \) remains the same.

Let us divide \( \mathcal{L} \) into a storage network \( \mathcal{S} \) and a retrieval measurement \( \mathcal{R} \), as shown in Fig. 5. We introduce the input space \( \mathcal{X}_i := \mathbb{O}_{i=1}^{N} \mathcal{H}_2^{(2k)} \) (denoted with numbers \( 2, 4, \ldots, 2N \) on Fig. 5) and the output space \( \mathcal{X}_O := \mathbb{O}_{i=1}^{N} \mathcal{H}_2^{(2k-1)} \) (denoted with numbers \( 1, 3, \ldots, 2N - 1 \) ). Additionally, we define spaces \( \mathcal{H}_2^{(in)} \), \( \mathcal{H}_2^{(out)} \) and \( \mathcal{H}_s \). The space \( \mathcal{H}_s \) has arbitrary dimension \( s \), but not smaller than the dimension of \( \mathcal{X}_i \otimes \mathcal{X}_O \). The storage \( \mathcal{S} \) can be realized as a sequence of isometry channels followed by a partial trace operation [28] Theorem 2.6]. Therefore, by moving the partial trace operation to the retrieval part, \( \mathcal{R} \), we may assume that the storage \( \mathcal{S} \) consists of an initial pure state followed by a sequence of isometry channels. In consequence, the Choi-Jamiołkowski matrix of \( \mathcal{S} \) has the form \( S = |X\rangle\langle X| \). There exists an isometry \( V \in M(\mathcal{H}_s, \mathcal{X}_i \otimes \mathcal{X}_O) \), such that \( X = \sqrt{\text{Tr}_{\mathcal{H}_s} S} V^\dagger \). In this notation, \( S \) is the solution of \( S = (\mathbb{I}_N \otimes V) / (\sqrt{\text{Tr}_{\mathcal{H}_s} S}) (\mathbb{I}_N \otimes V)^\dagger \). Hence, the isometry channel \( V \cdot V^\dagger \) can be treated as a postprocessing of the storage \( \mathcal{S} \) and also viewed as a part of the retrieval \( \mathcal{R} \). In summary, after all changes, the storage \( \mathcal{S} \) is of the

Figure 5: Schematic representation of the setup, which we use to upper bound \( F \). In this scenario, we are given \( N \) copies of unitary channel \( \Phi_{U,i} \) in parallel. Our objective is to approximate the von Neumann measurement \( \mathcal{P}_U \).
form  

\[ S = \left| \sqrt{\text{tr}_{\mathcal{H}_s} S} \right\rangle \langle \sqrt{\text{tr}_{\mathcal{H}_s} S} \right| \].  

By using the normalization property \[28, \text{Theorem 2.5}\] for the network presented in Fig. 6, we obtain  

\[ \text{tr}_{\mathcal{H}_s} \left( \mathbb{I}_2 \otimes \text{tr}_{\mathcal{H}_s} S \right) \right| \langle (\mathbb{I}_2 \otimes U)\otimes^N \text{tr}_{\mathcal{H}_s} S \rangle \left| \langle (\mathbb{I}_2 \otimes U)\otimes^N \right| \langle \mathbb{I}_2 \otimes^N \right| = 0 \]  

(B8)

Let us define the memory state  \( \sigma_{\Phi_{U_1}, S} \) as an application of the storage  \( S \) on  \( N \) copies of  \( \Phi_{U_1} \). Then, we have

\[
\sigma_{\Phi_{U_1}, S} = \text{tr}_{X_1 \otimes X_2} \left[ \left| \sqrt{\text{tr}_{\mathcal{H}_s} S} \right\rangle \langle \sqrt{\text{tr}_{\mathcal{H}_s} S} \right| \left( (\mathbb{I}_2 \otimes U)\otimes^N \text{tr}_{\mathcal{H}_s} S \right) \left| \langle (\mathbb{I}_2 \otimes U)\otimes^N \right| \right]  
\]

(B9)

where in the last equality we used the property Eq. (B8) and introduced  \( |\psi\rangle := \left( (\mathbb{I}_2 \otimes^N \otimes \mathbb{I}_4^N) | \sqrt{\text{tr}_{\mathcal{H}_s} S} \right) \). The above means that an arbitrary storage strategy  \( S \), which has access to  \( N \) copies of the unitary channel  \( \Phi_{U_1} \) can be replaced with parallel storage strategy of  \( N \) copies of a unitary channel  \( \Phi_{U_1} \). By exploiting this property to Eq. (B5) we obtain

\[
F \leq \frac{1}{2} \max_{\mathcal{L}} \int dU \text{tr} \left[ L^\top \left( (\mathbb{I}_2 \otimes U)J_{\Delta}(1 \otimes U^\top) \otimes (1 \otimes U^\top) #^N \right) \right]  
\]

(B10)

2. Objective function simplification

The aim of this section is to simplify the maximization of the fidelity function  \( F_p \) defined in Eq. (B3). Let us consider a binary measurement  \( \mathcal{R} = \{R_0, R_1\} \) taken from the maximization domain in Eq. (B3). It holds that  \( R_0 + R_1 = \mathbb{I}_{2N+1} \) and hence we may write

\[
F_p = \max_{\mathcal{R} = \{R_0, R_1\}} \int dU \frac{1}{2} \sum_{i=0}^1 \text{tr} \left[ R_i \left( (U \otimes \bar{U})\otimes^N \otimes \mathbb{I}_a \right) (|i\rangle\langle i| \otimes |\psi\rangle\langle \psi|)(U^\top \otimes U^\top \otimes^N \otimes \mathbb{I}_a) \right]  
\]

(B11)
where \( \sigma_z = |0\rangle\langle 0| - |1\rangle\langle 1| \). Taking the average of the matrix \( R_0 \) over the unitary group \( \{ U \otimes \bar{U} \otimes N \otimes I_n \} \) is equivalent to taking \( R \) such that \( 0 \leq R \leq 1_{2^{2N+1}} \) and \( [R, U \otimes \bar{U} \otimes N \otimes I_n] = 0 \) for any qubit unitary matrix \( U \). Equivalently, we may write \( [R^{opz}, U \otimes N + 1 \otimes I_n] = 0 \), where \( \bar{T} \) represents the partial transposition over subsystem \( Z \). According to \( \text{[34 Theorem 7.15]} \) the matrix \( R^{\bar{T}z} \) commutes with \( U \otimes N + 1 \otimes I_n \) if and only if it is of the form

\[
R^{\bar{T}z} = \sum_{\pi} W_\pi \otimes M_\pi, \tag{B12}
\]

where matrices \( W_\pi \in M(Z \otimes \mathcal{X}) \) represent subsystem permutation matrices acting on \( N + 1 \) qubit systems, according to the equation

\[
W_\pi |b_0, b_1, \ldots, b_N \rangle = |b_{\pi(0)}, b_{\pi(1)}, \ldots, b_{\pi(N)} \rangle, b_k \in \{0, 1\}. \tag{B13}
\]

The matrices \( M_\pi \) belong to the set \( M(Z) \) and the index \( \pi \) goes over all permutations of the set \( \{0, \ldots, N\} \). Hence, we may simplify calculation of \( F_p \)

\[
F_p = \frac{1}{2} + \frac{1}{2} \max_{0 \leq R \leq 1_{2^{2N+1}}} \max_{R = \sum_{\pi} W_\pi \otimes M_\pi} \frac{\langle \psi | R(\sigma_z \otimes |\psi\rangle |\psi\rangle \rangle}{\langle \psi | \psi \rangle \rangle} = \frac{1}{2} + \frac{1}{2} \max_{0 \leq R \leq 1_{2^{2N+1}}} \max_{R = \sum_{\pi} W_\pi \otimes M_\pi} \frac{\langle \psi | R \sigma_z \otimes |\psi\rangle |\psi\rangle \rangle}{\langle \psi | \psi \rangle \rangle} \tag{B14}
\]

To simplify the calculation of \( F_p \) even further, we introduce the following notation of basis states defined on \( N + 1 \) qubit system with fixed weight. We enumerate qubit subsystems with numbers \( 0, 1, \ldots, N \). For any subset \( A_k \subset \{1, \ldots, N\} \), such that \( |A_k| = k \), we define:

\[
\mathcal{H}_{2^N} \ni |A_k \rangle := \bigotimes_{i=1}^{N} (\delta(i \in A_k) |1\rangle + \delta(i \notin A_k) |0\rangle). \tag{B15}
\]

Consider the following subspaces of the \( N + 1 \) qubit space:

\[
\mathcal{H}^{(k)} := \text{span} (|0\rangle |A_k \rangle, |1\rangle |A_{k+1} \rangle : A_k, A_{k+1} \subset \{1, \ldots, N\}) \tag{B16}
\]

for \( k = -1, \ldots, N \), where the vectors exist only if the expression is well-defined (for instance, the vectors \( |A_{-1}\rangle, |A_{N+1}\rangle \) do not exist). In this notation, subspaces \( \mathcal{H}^{(k)} \) constitute a decomposition of \( N + 1 \) qubit space, \( \mathcal{H}_{2^{N+1}} = \bigoplus_{k=1}^{N} \mathcal{H}^{(k)} \). One may observe that the matrix \( R \) which appears in the maximization domain of Eq. \( \langle B14 \rangle \) is block diagonal in the introduced decomposition (in the partition \( Z \otimes \mathcal{X}/\mathcal{Y} \)). For such a \( R \), let us consider

\[
H_R = \text{tr}_Z (R(\sigma_z \otimes I_{2N})). \tag{B17}
\]

The matrix \( H_R \) is block diagonal in the decomposition

\[
\mathcal{H}_{2^N} = \bigoplus_{k=0}^{N} \text{span} (|A_k\rangle : A_k \subset \{1, \ldots, N\})). \tag{B18}
\]

Hence, we will write \( H_R \) as

\[
H_R = \bigoplus_{k=0}^{N} H_{R,k}. \tag{B19}
\]

Utilizing the above observations, the maximization problem Eq. \( \langle B14 \rangle \) can be written as

\[
F_p = \frac{1}{2} + \frac{1}{2} \max_{0 \leq R \leq 1_{2^{2N+1}}} \max_{R = \sum_{\pi} W_\pi \otimes M_\pi} \frac{\langle \psi | R(\sigma_z \otimes |\psi\rangle |\psi\rangle \rangle}{\langle \psi | \psi \rangle \rangle} = \frac{1}{2} + \frac{1}{2} \max_{0 \leq R \leq 1_{2^{2N+1}}} \max_{R = \sum_{\pi} W_\pi \otimes M_\pi} \lambda_1 (H_{R,k}) \tag{B20}
\]

where \( \lambda_1 (\cdot) \) stands for the largest eigenvalue and we used shortcut \( \mathbb{1} = 1_{2^{2N+1}} \). Finally, we observe that \( H_R = -\sigma_z^{\otimes N} \otimes I_n \) \( H_{R}(\sigma_z^{\otimes N} \otimes I_n) \), where \( \sigma_z = |0\rangle |1\rangle + |1\rangle |0\rangle \). It implies that \( H_{R,k} \) is unitarily equivalent to \( -H_{R,N-k} \) for any \( k \). We use this fact to write the final simplification of \( F_p \). The following lemma sums up all the considerations presented in this section.
Lemma 8. For the fidelity function $F_p$ defined in Eq. [B3], it holds that

$$F_p = \frac{1}{2} + \frac{1}{2} \max_{k=0, \ldots, \lfloor N/2 \rfloor} \max_{R: 0 \leq R \leq 1} \|H_{R,k}\|_{\infty}.$$  \hspace{1cm} (B21)

3. The upper bound on $F_p$ for $N = 1, 2$. 

In this subsection we will prove that Conjecture [B1] is true for $N = 1$ and $N = 2$. What is more, the presented proofs of Proposition [B21] and Proposition [B22] state a gentle introduction of ideas used in Subsection [B3]. We also find the upper bound for Eq. (B21) in the case $k = 0$, which supports the validity of Conjecture [B21] for $N > 2$.

Proposition 1. For matrices $R$ and $H_{R,0}$ defined in Subsection [B2] we have

$$\max_{R: 0 \leq R \leq 1} \|H_{R,0}\|_{\infty} \leq \frac{N}{N+1}. \hspace{1cm} (B22)$$

As a consequence, for $N = 1$ we get $F_p \leq \frac{3}{4}$.

Proof. Let us fix $R$ such that $0 \leq R \leq 1$ and $R = \sum_{\pi} W_{\pi}^T x \otimes M_{\pi}$. Note that

$$H_{R,0} = (\langle A_0 \rangle \otimes \mathbb{1}_a) R (\langle A_0 \rangle \otimes \mathbb{1}_a) = (\langle A_0 \rangle \otimes \mathbb{1}_a) \text{tr}_{2} [R (\sigma_x \otimes \mathbb{1}_{4^N})] (\langle A_0 \rangle \otimes \mathbb{1}_a)$$

$$= \sum_{\pi} M_{\pi} - \sum_{\pi(0) = 0} M_{\pi} - \sum_{\pi(0) \neq 0} M_{\pi}. \hspace{1cm} (B23)$$

From the assumption $0 \leq R \leq 1$, we have $0 \leq (\langle 1 \rangle \langle A_0 \rangle R (\langle 1 \rangle \langle A_0 \rangle) \mathbb{1}_a) \leq 1$, which is equivalent to

$$0 \leq \sum_{\pi(0) = 0} M_{\pi} \leq 1. \hspace{1cm} (B24)$$

Direct calculations reveal

$$\langle 0 \rangle (\langle A_0 \rangle \otimes \mathbb{1}_a) R (\langle 0 \rangle \langle A_0 \rangle) \mathbb{1}_a) = \sum_{\pi} M_{\pi},$$

$$\langle 0 \rangle (\langle A_0 \rangle \otimes \mathbb{1}_a) R (\langle 1 \rangle \langle j \rangle \mathbb{1}_a) = \sum_{\pi(0) = j} M_{\pi}, \hspace{1cm} (B25)$$

$$\langle 1 \rangle (\langle i \rangle \otimes \mathbb{1}_a) R (\langle 1 \rangle \langle j \rangle \mathbb{1}_a) = \sum_{\pi(0) = 0, \pi(i) = j} M_{\pi} + \sum_{\pi(0) = j, \pi(i) = 0} M_{\pi}.$$

Let us define a unit vector $|x\rangle = 1/\sqrt{N^2 + N} (N \langle 0 \rangle \langle A_0 \rangle \mathbb{1}_a) + \sum_{i} |\langle i \rangle \rangle$. We obtain

$$\langle x \rangle (\mathbb{1}_a) R (\langle x \rangle \otimes \mathbb{1}_a) = \frac{1}{N^2 + N} \left( \sum_{\pi(0) = i} M_{\pi} + \sum_{\pi(i) = 0} M_{\pi} \right) + \sum_{i,j} \left( \sum_{\pi(0) = 0, \pi(i) = j} M_{\pi} + \sum_{\pi(0) = j, \pi(i) = 0} M_{\pi} \right). \hspace{1cm} (B26)$$

By $0 \leq \langle x \rangle (\mathbb{1}_a) R (\langle x \rangle \otimes \mathbb{1}_a) \leq 1$ we have

$$0 \leq \langle x \rangle (\mathbb{1}_a) R (\langle x \rangle \otimes \mathbb{1}_a) = \frac{1}{N^2 + N} \left( \sum_{\pi(0) = 0} M_{\pi} + (N + 1)^2 \sum_{\pi(0) \neq 0} M_{\pi} \right) \leq 1. \hspace{1cm} (B27)$$

Combining inequalities Eq. (B24) and Eq. (B27) we get

$$\|H_{R,0}\|_{\infty} \leq \frac{N}{N+1}, \hspace{1cm} (B28)$$

\qed
Proposition 2. For $N = 2$ and $F_p$ defined in Eq. (B21) we have $F_p \leq \frac{5}{6}$.

Proof. Let us fix $R$ such that $0 \leq R \leq 1$ and $R = \sum_\pi W^{T,z}_\pi \otimes M_\pi$. We will show that $\|H_{R,1}\|_\infty < \frac{2}{3}$, which immediately implies $F_p \leq \frac{5}{6}$. Let us define two orthogonal vectors

\[
\begin{align*}
|\xi_0\rangle &= 2|001\rangle - |010\rangle + 2|111\rangle \in \mathcal{H}_8, \\
|\xi_1\rangle &= -|001\rangle + 2|010\rangle + 2|111\rangle \in \mathcal{H}_8
\end{align*}
\] (B29)

and an isometry operator $I$ given as $I = (|\xi_0\rangle\langle 0| + |\xi_1\rangle\langle 1|)/3$. We can focus on two distinct classes of permutations $\pi$ of the set $\{0, 1, 2\}$: rotations $r_0 = (0)(1)(2)$, $r_1 = (0, 1, 2)$, $r_2 = (0, 2, 1)$ and symmetries $s_0 = (1, 2)$, $s_1 = (0, 2)$, $s_2 = (0, 1)$. In this notation we have

\[
H_{R,1} = \begin{bmatrix}
M_{s_2} - M_{s_1} & M_{s_2} - M_{r_1} \\
M_{r_1} - M_{r_2} & M_{s_1} - M_{s_2}
\end{bmatrix}.
\] (B30)

One can calculate that

\[
9(I^\dagger \otimes \mathbb{1}_4)R(I \otimes \mathbb{1}_4) = \begin{bmatrix}
9M_{r_0} + 4M_{r_1} + 16M_{r_2} & 9M_{r_1} + 16M_{r_2} \\
9M_{r_0} + 4M_{r_1} + 16M_{r_2} & 9M_{r_2} + 16M_{r_2} + 4M_{s_2} + 16M_{s_2} + 4M_{s_2}
\end{bmatrix}.
\] (B31)

Hence, we obtain

\[
9(I^\dagger \otimes \mathbb{1}_4)R(I \otimes \mathbb{1}_4) - 9(\sigma_x I^\dagger \otimes \mathbb{1}_4)R(I \otimes \mathbb{1}_4) = 15 \begin{bmatrix}
M_{s_2} - M_{s_1} & M_{r_2} - M_{r_1} \\
M_{r_1} - M_{r_2} & M_{s_1} - M_{s_2}
\end{bmatrix} = 15H_{R,1}.
\] (B32)

From the assumptions, we have $0 \leq (I^\dagger \otimes \mathbb{1}_4)R(I \otimes \mathbb{1}_4) \leq \mathbb{1}$ and finally we obtain

\[
\|H_{R,1}\|_\infty \leq \frac{3}{5} < \frac{2}{3}.
\] (B33)

\[\square\]

4. Technical lemmas

In the following lemma we will observe that optimization problem in Eq. (B21) can be reduced to the case $k \in \mathbb{N}, N = 2k$.

Lemma 9. Let $N \in \mathbb{N}$ and take $k$, such that $k \leq N/2$. It holds that

\[
\max_{\bar{R} = \sum_\pi W^{T,z}_\pi \otimes M_\pi} \max_{0 \leq R \leq 1} \|H_{R,k}\|_\infty \leq \max_{\bar{R} = \sum_\pi \tilde{W}^{T,z}_\pi \otimes \tilde{M}_\pi} \|\tilde{H}_{\bar{R},N-k}\|_\infty,
\] (B34)

where the matrix $\bar{R}$ is defined for $\bar{N} = 2(N-k)$ and hence the number of systems on which the matrix $\tilde{W}_\pi$ acts is $\bar{N} + 1$.

Proof. Let us fix $R$ such that $0 \leq R \leq \mathbb{1}$ and $R = \sum_\pi W^{T,z}_\pi \otimes M_\pi$. Define

\[
\bar{R} := \sum_\pi \left(W^{T,z}_\pi \otimes \mathbb{1}_{2^{N-2k}}\right) \otimes \left(M_\pi \otimes \mathbb{1}_{2^{N-2k}}\right).
\] (B35)

We see that matrix $\bar{R}$ is in the maximization domain of the right-hand side of Eq. (B34). Then, we have $\tilde{H}_{\bar{R}} = \text{tr}_{\bar{z}} \left(\tilde{R}(\sigma_z \otimes \mathbb{1})\right) = \mathbb{1}_\bar{N}, \tilde{H}_{\bar{R},1}$. The matrix $\tilde{H}_{\bar{R},N-k}$ is defined on the space spanned by the vectors $|A_{N-k}\rangle \in \mathcal{H}_{2N}$ for $A_{N-k} \subseteq \{1, \ldots, \bar{N}\}$. These vectors can be expressed in the form $|A_{N-k}\rangle = |B_i\rangle |B_{N-k-i}\rangle$, where $|B_i\rangle \in \mathcal{H}_{2N}$ for $B_i$ such that $|B_i| = i$, $B_i \subseteq \{1, \ldots, \bar{N}\}$, and $|B_{N-k-i}\rangle \in \mathcal{H}_{2^{N-2k}}$, $B_{N-k-i} \subseteq \{N+1, \ldots, \bar{N}\}$. Then, we have

\[
\langle (A_{N-k} \otimes \mathbb{1}) \tilde{H}_{\bar{R},N-k} (A'_{N-k} \otimes \mathbb{1}) \rangle = \langle B_{N-k-i} B'_{N-k-i} \rangle (\langle B_i \rangle \otimes \mathbb{1}) H_R (|B'_i\rangle \otimes \mathbb{1}) \otimes \mathbb{1}.
\] (B36)
The non-zero blocks exist if and only if \( i = i' \) and \( B_{N-k-i} = B'_{N-k-i'} \), so

\[
\tilde{H}_{R,N-k} = \bigoplus_{i=k}^{N-k} \bigoplus_{B_{N-k-i} \subseteq \{N+1, \ldots, \tilde{N}\}} H_{R,i} \otimes \mathbb{I}.
\]

(B37)

That means

\[
\|\tilde{H}_{R,N-k}\|_\infty = \max_{i=k, \ldots, N-k} \|H_{R,i}\|_\infty \geq \|H_{R,k}\|_\infty.
\]

(B38)

In the next lemma we will find the upper bound for Eq. (B21) in the case \( N = 2k \) for \( k \in \mathbb{N} \).

**Lemma 10.** Let \( k \in \mathbb{N} \) and \( N = 2k \). For matrices \( R \) and \( H_{R,k} \) defined in Subsection B2 we have

\[
\max_{R: 0 \leq R \leq 1} \|H_{R,k}\|_\infty \leq 1 - \Theta \left( \frac{1}{k^2} \right).
\]

(B39)

**Proof.** Let us fix \( R \) such that \( 0 \leq R \leq 1 \) and \( R = \sum_{\pi} W^T_{\pi} \otimes M_\pi \). Through the rest of the proof, by \( B_i \) we denote subsets of \( \{1, \ldots, 2k\} \), such that \( |B_i| = l \), for \( l = 0, \ldots, 2k \). Following the notation introduced in Subsection B2 we define four types of vectors:

1. \( |+_{A_k} \rangle = x \langle 0 | A_k \rangle + \sum_{B_{k+1}: |B_{k+1} \cap A_k| = k} |1 \rangle \langle B_{k+1}| \)
2. \( |-_A \rangle = x |1 \rangle \langle A_k \rangle + \sum_{B_{k-1}: |B_{k-1} \cap A_k| = k-1} |0 \rangle \langle B_{k-1}| \)
3. \( |\oplus_{A_k} \rangle = \sum_{|B_{k+1}: |B_{k+1} \cap A_k| = 1} |1 \rangle \langle B_{k+1}| \)
4. \( |\ominus_{A_k} \rangle = \sum_{|B_{k-1}: |B_{k-1} \cap A_k| = 0} |0 \rangle \langle B_{k-1}| \)

for each \( A_k \subset \{1, \ldots, 2k\} \) and some \( x > 0 \). Now we define the following matrices:

1. \( I_+ = \sum_{A_k} |+_{A_k}\rangle \langle A_k| \)
2. \( I_- = \sum_{A_k} |-_A \rangle \langle A_k| \)
3. \( I_\oplus = \sum_{A_k} |\oplus_{A_k} \rangle \langle A_k| \)
4. \( I_\ominus = \sum_{A_k} |\ominus_{A_k} \rangle \langle A_k| \)

For arbitrary \( A_k, A'_k \subset \{1, \ldots, 2k\} \) we have

1. \( \langle +_{A_k}| +_{A'_k} \rangle = x^2 \delta(A_k = A'_k) + \{|B_{k+1}: |B_{k+1} \cap A_k| = k, |B_{k+1} \cap A'_k| = k\} \)
2. \( \langle -_{A_k}| -_{A'_k} \rangle = x^2 \delta(A_k = A'_k) + \{|B_{k-1}: |B_{k-1} \cap A_k| = k-1, |B_{k-1} \cap A'_k| = k-1\} \)
3. \( \langle \oplus_{A_k}| \oplus_{A'_k} \rangle = \{|B_{k+1}: |B_{k+1} \cap A_k| = 1, |B_{k+1} \cap A'_k| = 1\} \)
4. \( \langle \ominus_{A_k}| \ominus_{A'_k} \rangle = \{|B_{k-1}: |B_{k-1} \cap A_k| = 0, |B_{k-1} \cap A'_k| = 0\} \).
We can observe that if \( A_k = A'_k \), then the above inner products are \( x^2 + k, x^2 + k, k, k \), respectively. If \( |A_k \cap A'_k| = k - 1 \) then all the inner products are equal to one. Finally, if \( |A_k \cap A'_k| < k - 1 \) then we obtain all the inner products are equal to zero. We note two useful facts about matrices \( I_+, I_-, I_{\oplus}, I_{\ominus} \). Firstly, we have

\[
I^\dagger_+ I_+ + I^\dagger_{\ominus} I_{\ominus} = I^\dagger_- I_- + I^\dagger_{\oplus} I_{\oplus}.
\]

(B40)

Secondly, one can show that

\[
\|I^\dagger_+ I_+ + I^\dagger_{\ominus} I_{\ominus}\|_\infty = x^2 + 2k + 2k^2.
\]

(B41)

As far as the first equality is straightforward, to show the second one, note that for each \( A_k \) there is exactly \( k^2 \) sets \( A'_k \) such that \( |A_k \cap A'_k| = k - 1 \). This means that by Birkhoff’s Theorem we can express \( I^\dagger_+ I_+ + I^\dagger_{\ominus} I_{\ominus} \) in the basis given by vectors \( |A_k\rangle \) as \( I^\dagger_+ I_+ + I^\dagger_{\ominus} I_{\ominus} = (x^2 + 2k) \mathbb{1} + 2 \sum_{i=1}^{k^2} \Pi_i \), where \( \Pi_i \) are permutation matrices. By the triangle inequality we have that the spectral norm is no greater than \( x^2 + 2k + 2k^2 \). By taking the normalized vector \( |x\rangle \propto \sum A_k |A_k\rangle \) we get \( \langle x | \left( I^\dagger_+ I_+ + I^\dagger_{\ominus} I_{\ominus} \right) |x\rangle = x^2 + 2k + 2k^2 \).

To state the upper bound for \( \|H_{R,k}\|_\infty \) we will use the definition of \( H_R \) from Eq. (B17) and the decomposition from Eq. (B19). For a given \( A_k, A'_k \subset \{1, \ldots, 2k\} \) we have that

\[
\langle A_k \otimes I_a | H_{R,k} (|A'_k\rangle \otimes I_a) \rangle = \sum_{\pi : (A_k) = A'_k} M_{\pi} - \sum_{\pi : (0, A_k) = 0, A'_k} M_{\pi} = \sum_{\pi : (0) \neq 0, \pi : (A_k) = A'_k} M_{\pi} - \sum_{\pi : (0) \neq 0, \pi : (0, A_k) = 0, A'_k} M_{\pi}.
\]

(B42)

Let us now define

\[
G_{R,k} = (I^\dagger_+ \otimes I_a) R(I_+ \otimes I_a) + (I^\dagger_{\ominus} \otimes I_a) R(I_{\ominus} \otimes I_a) - (I^\dagger_- \otimes I_a) R(I_- \otimes I_a) - (I^\dagger_{\oplus} \otimes I_a) R(I_{\oplus} \otimes I_a).
\]

(B43)

Taking \( A_k, A'_k \subset \{1, \ldots, 2k\} \) we have:

\[
\langle A_k \otimes I_a | G_{R,k} (|A'_k\rangle \otimes I_a) \rangle
\]

\[
= \begin{pmatrix}
  x^2 \sum_{\pi : (A_k) = A'_k} M_{\pi} + x \sum_{B_{k+1}^\prime, \pi : |B_{k+1}^\prime \cap A'_k| = k, \pi (0, A_k) = B_{k+1}^\prime} M_{\pi} + x \sum_{B_{k+1}^\prime, \pi : |B_{k+1}^\prime \cap A_k| = k, \pi (B_{k+1}) = 0, A'_k} M_{\pi} + \sum_{B_{k+1}^\prime, B_{k-1}^\prime, \pi : |B_{k+1}^\prime \cap A'_k| = k - 1, \pi (A_k) = 0, B_{k-1}^\prime} M_{\pi} \\
  x^2 \sum_{\pi : (0, A_k) = 0, A'_k} M_{\pi} + x \sum_{B_{k-1}^\prime, \pi : |B_{k-1}^\prime \cap A'_k| = k - 1, \pi (A_k) = B_{k-1}^\prime} M_{\pi} + x \sum_{B_{k-1}^\prime, \pi : |B_{k-1}^\prime \cap A_k| = k - 1, \pi (0, B_{k-1}) = A'_k} M_{\pi} + \sum_{B_{k-1}^\prime, B_{k+1}^\prime, \pi : |B_{k-1}^\prime \cap A'_k| = k - 1, \pi (B_{k-1}) = B_{k+1}^\prime} M_{\pi}
\end{pmatrix}
\]

(B44)
This can be simplified to
\[
(A_k \otimes 1_a) G_{R,k} (A'_k \otimes 1_a) = \left( \sum_{\pi: \pi(A_k) = A'_k} \sum_{B_{k+1} \subseteq \pi: \pi(B_{k+1} \cap A_k) = k,} \sum_{\pi(0, A_k) = B_{k+1}} M_\pi \right) + \left( \sum_{\pi: \pi(0, A_k) = 0, A'_k} \sum_{B_{k+1} \subseteq \pi: \pi(B_{k+1} \cap A_k) = k-1,} \sum_{\pi(0, A_k) = 0, B_{k-1}} M_\pi \right)
\]
(B45)

Let us write the above as \(((A_k \otimes 1_a) G_{R,k} (A'_k \otimes 1_a) = \sum_\pi c_\pi M_\pi\), where \(c_\pi\) are some constants. For each \(\pi\), let us determine the value of \(c_\pi\):
- For \(\pi\) such that \(\pi(0) = 0, \pi(A_k) = A'_k\) we have \(c_\pi = x^2 - x^2 = 0\).
- For \(\pi\) such that \(\pi(0) = 0, \pi(A_k) \neq A'_k\) we have \(c_\pi = 0\).
- For \(\pi\) such that \(\pi(0) \neq 0, \pi(A_k) = A'_k\) we have \(c_\pi = x^2 + x + x = x^2 + 2x\).
- For \(\pi\) such that \(\pi(0) \neq 0, \pi(A_k) \neq A'_k, \pi(0, A_k) \neq 0, A'_k\) there exists \(a_0 \notin \{0\} \cup A_k\), such that \(\pi(a_0) \in \{0\} \cup A'_k\).

Therefore, we consider two sub-cases:
- If for each \(a \notin \{0\} \cup A_k\) it holds \(\pi(a) \notin A'_k\), then \(\pi(a_0) = 0, \pi(0) \in A'_k\) and \(A'_k \subset \pi(0, A_k)\). Then, \(c_\pi = x - x = 0\).
- If \(\pi(a_0) \in A'_k\), then we have two options:
  * If \(\pi(a_0, A_k) = 0, A'_k\), then \(c_\pi = x - x = 0\).
  * If \(\pi(a_0, A_k) \neq 0, A'_k\), then \(c_\pi = 0\).

Therefore, we can see that \(G_{R,k} = (x^2 + 2x)H_{R,k}\). Then, utilizing Eq. (B40), Eq. (B41) and Eq. (B43) we get
\[
-(x^2 + 2k \leq x^2 + 2k) \leq G_{R,k} \leq x^2 + 2k + 2k^2)
\]
and finally we obtain \(\|H_{R,k}\|_\infty \leq \frac{x^2 + 2k + 2k^2}{x^2 + 2k}\). Minimizing over \(x \geq 0\), we get for \(x \approx 2k^2\) that \(\|H_{R,k}\|_\infty \leq 1 - \Theta(1/k^2)\), which finishes this case of the proof.

5. Proof of Lemma 1

Proof of Lemma 1 We have the following sequence of conclusions
\[
F \leq F_p \leq \frac{1}{2} + \frac{1}{2} \max_{k=0, \ldots, N/2} \|H_{R,k}\|_\infty \quad \text{(by Eq. (B2), Eq. (B3), Lemma 7)}
\]
(\text{by Lemma 8})
\[
\leq \frac{1}{2} + \frac{1}{2} \max_{k=0, \ldots, N/2} \|\tilde{H}_{R,N-k}\|_\infty \quad \text{(by Lemma 9)}
\]
\[
\leq \frac{1}{2} + \frac{1}{2} \max_{k=0, \ldots, N/2} 1 - \Theta \left( \frac{1}{(N-k)^2} \right) \quad \text{(by Lemma 10)}
\]
\[
eq 1 - \Theta \left( \frac{1}{N^2} \right).
\]