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Estimation of Potentially Unphysical Maps

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Abstract. When standard methods of process (black-box) estimation are applied straightforwardly then it may happen that some sets of experimental data result in unphysical estimations of the corresponding channels (maps) describing the process. To prevent this problem, one can use the method of maximum likelihood (MML), which provides an efficient scheme for reconstruction of quantum channels. This scheme always results in estimations of channels that are fully physical, e.g. the corresponding maps are linear, positive and completely positive. To show this property, we use the MML for a derivation of physical approximations of truly unphysical operations. In particular, we analyze physical approximations of the universal-NOT gate, the quantum nonlinear polarization rotation and the map $\rho \longrightarrow \rho^2$. Given the result of MML, we examine retrospectively the quality of the experiment. Depending on the resulting value of the MML functional we can determine (physical) consistency of the input data.

1. Introduction

The task of a process reconstruction is to determine an unknown quantum channel (a "black box") using correlations between known input states and results of measurements performed on the states that have been transformed by the channel (see Fig. 1). The linearity of quantum dynamics implies that the channel $\mathcal{E}$ is exhaustively described by its action $\varrho_j \to \varrho'_j = \mathcal{E}[\varrho_j]$ on a set of basis states, i.e. a collection of linearly independent states ϱ_j, that play a role of *test states*. Therefore, to perform the reconstruction of channel $\mathcal{E}$ we have to perform a complete state tomography [1−5] of ϱ'_j. The number of test states equals d^2, where $d = \dim \mathcal{H}$ is the dimension of the Hilbert space associated with the system. Consequently, in order to reconstruct a channel we have to determine $d^2(d^2-1)$ real parameters, i.e. 12 numbers in the case of a qubit ($d = 2$).

In our previous paper [6] we have analyzed the the possibility of using the method of *maximum likelihood* (MML) [7] (for a review see e.g. [8]) to perform an estimation of an unknown channel. We used this method to perform the reconstruction based on numerical simulation of the anti-unitary universal-NOT (U-NOT) gate [9, 10]. This is a linear, but not a CP map and we showed how our regularization methods results in the optimal physical approximations of the

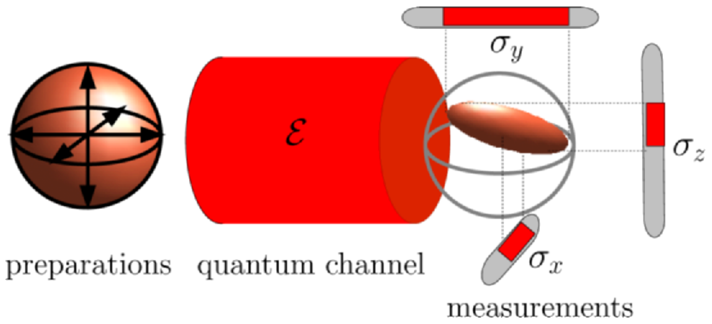

Fig. 1: Schematic representation of the reconstruction of a single-qubit channel. Input (test) states of single-qubit channels are represented by the Bloch sphere (the state space of a single qubit). On the output of the channel (modelled as an ellipsoid, i.e. the Bloch sphere that is "deformed" by the channel action) a complete measurement of test states is performed, via the projective measurement of σ operators. Based on the correlations between input and output states of test qubits, the action of the quantum channel (CP map) is determined or estimated.

U-NOT operation. In order to demonstrate the power of this approach we also applied it to obtain an approximation of nonlinear quantum-mechanical map — the so called *nonlinear polarization rotation* (NPR) [11]. In this paper we will examine another highly nonlinear transformation $\rho \longrightarrow \rho^2$. We will present the best physical approximation of this nonlinear map.

Having the result of MML method, one has to determine how reliable this result is. As any numerical method, MML may fail by falling to (or rather climbing up to) a nonlocal maxima. On the other hand, data provided by experiment may lead to unphysical results. In this case it is not surprising that any physical approximation based on inconsistent data will result in an inconsistent map, e.g. a map that does not reproduce the experimental data perfectly. To deal with such cases, we will examine the resulting value of the MML functional. We will show that in certain cases it may be used as an indicator of physical consistency of the input data.

Our paper is organized as follows: In Sect. 2 we briefly describe basic properties of single-qubit channels. In Sect. 3 we show how the method of maximum likelihood can be applied for an estimation of quantum channels on three examples: the universal-NOT gate, the nonlinear polarization rotation and the map $\rho \longrightarrow \rho^2$. In Sect. 4 we will examine, how to use the value of the MML functional to detect the quality/consistency of the input data.

2. Method of Maximum Likelihood

The MML is a general estimation scheme [7, 8] that has already been considered for a reconstruction of quantum operations from incomplete data. Given the measured data represented by couples ϱ_k, F_k (ϱ_k is one of the test states and F_k is a positive operator corresponding to the outcome of the measurement used in the k-th run of the experiment) the likelihood functional is defined by the formula

$$L(\mathcal{E}) \;=\; -\log \prod_{k=1}^{N} p(k|k) \;=\; -\sum_{k=1}^{N} \log \mathrm{Tr}\, \mathcal{E}[\varrho_k] F_k \,, \tag{1}$$

where N is the total number of "clicks" and we used $p(j|k) = \mathrm{Tr}\, \mathcal{E}[\varrho_k] F_j$ for conditional probability of using test state ϱ_k and observe the outcome F_j. The aim is to find a physical map $\mathcal{E}_{\mathrm{est}}$ that maximizes this function, i.e. $L(\mathcal{E}_{\mathrm{est}}) = \max_{\mathcal{E}} L(\mathcal{E})$. This variational task is usually performed numerically.

Our approach differs from the method described in [12, 13, 14] in the way how we find the maximum of the functional defined by (1). The parametrization of $\mathcal{E}$ itself guarantees the trace-preserving condition. Hence only the CP condition must be checked separately during the numerical maximalization. Instead of using the Lagrange multipliers (and increasing thereby the number of parameters for the numerical procedure), we introduce the CP condition as an external boundary for a Nelder-Mead simplex algorithm. The maximalization itself is performed by Mathematica 5.0 build-in function with the following parameters:

- Method = Nelder Mead. We chose the *Simplex algorithm* because it gives the most stable results with the smallest memory requirements.
- Shrink ratio and Contract ratio = 0.95. These parameters are normally taken somewhere around 0.5. Their values close to unity induce a rather slow "cooling" of the process and prevents it from falling into a local maximum. So the global maximum can be determined reliably. The price to pay is, as usual, longer time of numerical search.
- Reflect ratio = 1.5. This parameter is bigger than the standard choice but it helps us to enhance the probability of finding the global maximum.

In the subsections below we shortly recall the analysis of the U-NOT and NPR operations and we discuss the $\rho \longrightarrow \rho^2$ operation.

2.1. U-NOT Gate

The logical NOT operation can be generalized into the quantum domain as a unitary transformation $|0\rangle \rightarrow |1\rangle$, $|1\rangle \rightarrow |0\rangle$. However, this map is basis dependent and does not transform all qubit states $|\psi\rangle$ into their (unique) orthogonal complements $|\psi_\perp\rangle$. Such *universal NOT* ($\mathcal{E}_{\mathtt{NOT}} : |\psi\rangle \rightarrow |\psi_\perp\rangle$) is associated with the inversion of the Bloch sphere, i.e. $\vec{r} \rightarrow -\vec{r}$, which is not a CP map. It represents an unphysical transformation specified by $\lambda_1 = \lambda_2 = \lambda_3 = -1$. This map is the most unphysical map among linear transformations of a single qubit and can be performed only approximatively. A quantum "machine" that optimally implements an approximation of the universal NOT has been introduced in [9, 15, 16] and experimentally realized by de Martini et al., [10]. The machine is represented by a map $\tilde{\mathcal{E}}_{\texttt{NOT}} = \mathrm{diag}\{1, -1/3, -1/3, -1/3\}$. The distance between the U-NOT and its optimal physical approximation reads

$$d(\tilde{\mathcal{E}}_{\texttt{NOT}}, \mathcal{E}_{\texttt{NOT}}) \;=\; \int_{\text{states}} \mathrm{d}\varrho \,\mathrm{Tr}\,|(\mathcal{E}_{\texttt{NOT}} - \tilde{\mathcal{E}}_{\texttt{NOT}})[\varrho]| \;=\; 1/3\,. \tag{2}$$

The map $\tilde{\mathcal{E}}_{\texttt{NOT}}$ corresponds to the best CP approximation of the universal-NOT operation, i.e. to the *optimal U-NOT gate*.

For the *Gedanken* experiment reconstruction of U-NOT gate we choose as an input the eigenstates of operators $\sigma_x, \sigma_y, \sigma_z$, that is we consider a set of six test states. The data are generated as (random) results of three projective measurements $\sigma_x, \sigma_y, \sigma_z$ applied in order to perform the output state reconstruction. For $N = 100 \times 18$ measurement records ("clicks"), i.e. each measurement is performed 100 times per particular input state, the MML algorithm results in the map

$$\mathcal{E}_{\text{est}} \;=\; \begin{pmatrix} 1 & 0 & 0 & 0 \\ -0.0002 & -0.3316 & -0.0074 & 0.0203 \\ 0.0138 & -0.0031 & -0.3334 & 0.0488 \\ -0.0137 & 0.0298 & -0.0117 & -0.3336 \end{pmatrix}, \tag{3}$$

which is very close $[d(\mathcal{E}_{\text{est}}, \mathcal{E}_{\text{app}}) = 0.0065]$ to the best approximation of the U-NOT operation, i.e. $\mathcal{E}_{\text{app}} = \mathrm{diag}\{1, -1/3, -1/3, -1/3\}$.

We conclude that for sufficiently large N the MML reconstruction gives us the same result as a theoretical prediction derived in [9]. In order to illustrate the power of this approach we will find approximations of nonlinear "quantum" mechanical transformations.

2.2. Nonlinear polarization rotation

Let us consider a nonlinear transformation of a qubit [11] defined by the relation

$$\mathcal{E}_\theta[\varrho] \;=\; e^{i\frac{\theta}{2}\langle\sigma_z\rangle_\varrho \sigma_z}\,\varrho\, e^{-i\frac{\theta}{2}\langle\sigma_z\rangle_\varrho \sigma_z}. \tag{4}$$

Unlike the universal-NOT which in linear though not a CP map the NPR is a nonlinear map. Four test states are not sufficient to allow us to determine the action of nonlinear maps. Consequently, the *Gedanken* measurement data must contain all possible input states (covering the whole Bloch sphere) as test states. Nevertheless, it is enough to use only three different measurements performed on outcomes. These measurements are sufficient for the reconstruction procedure.

We plot the parameter λ that specifies the best physical approximation of the NPR map in Fig. 2. In the same figure we also present a result of the maximum likelihood estimation of the NPR map based on a finite number of "measurements". Here, for every point (θ), the nonlinear operation was applied to

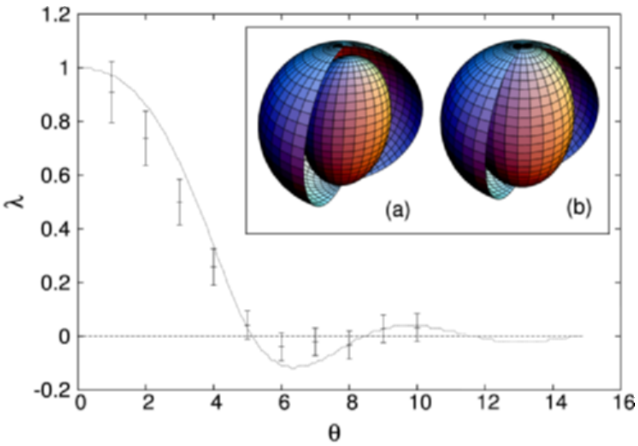

Fig. 2: We present analytical as well as numerical results of an approximation of the nonlinear map $\mathcal{E}_\theta$ given by (4) for different values of the parameter θ (measured in radians). The numerical ("experimental") results shown in the graph in terms of a set of discrete points with error bars are obtained via the MML. The theoretical approximation of the nonlinear NPR map is characterized by the parameter λ that is plotted (solid line) in the figure as a function of the parameter θ. In the inset (a) is the Bloch sphere transformation for $\theta = 3$ obtained by MML and in (b) the same transformation obtained analytically.

1800 input states that have been chosen randomly (via a Monte Carlo method). These input states have been transformed according to the nonlinear transformation (4). Subsequently simulations of random projective measurements have been performed. With these "experimental" data a maximization procedure was performed as described in the previous section.

2.3. Nonlinear transformation $\rho \longrightarrow \rho^2$

Similar to the previous example, the map $\rho \longrightarrow \rho^2$ is intrinsically nonlinear and we have to define the map for all possible inputs. The most general state of a qubit can be written as $\rho(\vec{r}) = 1/2(\mathbb{1} + \vec{r}\cdot\vec{\sigma})$ where $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ are Pauli matrices and $\vec{r}$ is a real vector and $|\vec{r}| \leq 1$. In such notation we can define the map as follows:

$$\mathcal{E}(\rho) = \frac{1}{2}\left(\mathbb{1} + |\vec{r}|\,\vec{r}\cdot\vec{\sigma}\right) \;=\; |\vec{r}|\rho + \frac{1}{2}\left(1 - |\vec{r}|\right)\mathbb{1}\,. \tag{5}$$

Since the action of the map cannot be written as a matrix independent of ρ acting on ρ, the map is not linear. Hence this map is a very interesting example for studying reconstruction schemes, as it does not change typical test states (pure states and the complete mixture state).

Due to the high symmetry of the map one would expect that the best physical approximation is a contraction of the whole Bloch sphere with a specific coefficient k,

$$\mathcal{E}(\rho)_{\text{physical}} \; = \; k\rho + \frac{1}{2}\,(1-k)\,\mathbb{1}\,, \tag{6}$$

with $0 \leq k \leq 1$. Indeed, the result of the MML method takes, within the precision given by finite number of test-states, the expected form

$$\mathcal{E}(\rho)_{\text{physical}} \; = \; 0.85\,\rho + \frac{1}{2}\,(1-0.85)\,\mathbb{1}\,. \tag{7}$$

Comparison with different analytical solutions (all using the symmetry of the operation, but with different distance measures on the space of one-qubit operations) will be presented in a separate paper.

3. Analysis of the Results

Using three examples presented in the previous section we have demonstrated the power of the MML method to find physical approximations of operations that are truly unphysical. In reality (when analyzing data of real experiments) one always expects to have physical operations. However, if data indicate an unphysical operation, this can be a consequence of experimental errors or a wrong interpretation of the measured data, but also it can indicate the failure of reconstruction method.

To rule out the last possibility, one always has to analyze precisely the outcome of the procedure. By performing the maximization numerically, the functional itself is a rather simple function of the input data. The only challenge are boundary conditions imposed by the CP requirement. These may cause the search-engine to get stuck in a point of a parameter space which is not a local maximum of the functional, but is confined by the boundary conditions. This case is easy to detect by calculating the CP condition of the resulting operation and to check if the result is on the boundary of the CP maps. If so, we run the maximization procedure again with different starting conditions. However, for parameters of the maximization procedure specified in Sect. 2, for every testing case the MML resulted in the proper maxima in the first attempt.

If the result of the MML method is correct and the resulting operation is yet on the boundary of CP maps, there is a strong evidence that the incoming data were biased by some kind of errors. To analyze this problem closer, we have to take into account not only the resulting operations, but also the value of the maximum likelihood functional L in (1). This value defines the logarithm of the probability to obtain, for specified input states (used in the MML method as test states), the same results as the experimental ones. For proper data, this probability should be comparable to probability of a sequence of measured data produced directly by the reconstructed operation. However, for physically inconsistent data (in our examples these data are produced by unphysical operations) the reconstructed operations may reproduce these data with much smaller probability.

	$L_{\text{data}}(\mathcal{E})$	$\bar{L}_{\text{test}}(\mathcal{E})$	$\sigma(L_{\text{test}}(\mathcal{E}))$
U NOT	-1371	-1472	6.79
NPR	-1423	-1426	12.64
$\rho \longrightarrow \rho^2$	-1343	-1335	17.44

Table 1: Values of the functional L for different examples of unphysical operations. For the first example (the universal-NOT gate) it is clear that the probability to obtain sequence similar to the sequence given by the experimental data is much lower than to obtain a typical sequence of data produced by the reconstructed operation. For the last two examples the difference is not significant.

We define the $L_{\text{data}}(\mathcal{E})$ to be the value of the functional (1) for the resulting approximation. For the same set of test states as used in the original experiments (denoted by ρ_k) we perform the *Gedanken* experiment. We apply the reconstructed operation on every such state and then apply the measurement in the same direction as in the original experiment (the resulting positive operators are denoted $\bar{F}_k$). Then we define

$$L_{\text{test}}(\mathcal{E}) \;=\; -\sum_{k=1}^{N} \log \operatorname{Tr} \mathcal{E}[\varrho_k]\bar{F}_k \,. \tag{8}$$

The same procedure can be repeated sufficiently many times to obtain a typical value of the functional (calculated as the mean of all runs and denoted by $\bar{L}_{\text{test}}(\mathcal{E})$) and the typical variance of this value $\sigma(L_{\text{test}}(\mathcal{E}))$.

In Table 1 results of the calculations for three examples analyzed in the previous section are presented. As one can clearly see, for the universal-NOT gate the difference between $L_{\text{data}}(\mathcal{E})$ and $\bar{L}_{\text{test}}(\mathcal{E})$ is rather big, providing a clear evidence that the input data originated from an unphysical operation. This is, however, not the case for the nonlinear polarization rotation and for the transformation $\rho \longrightarrow \rho^2$. In the latter two cases the typical sequence (as a whole) of the experimental data has a comparable probability to appear as any other sequence produced by the reconstructed operation. So we may conclude that this method gives us a partial tool (a necessary condition) to identify data that would lead to unphysical operations. A more complete analysis, which includes evaluation of sub-sequences of input data will be analyzed in a separate paper [17].

4. Conclusions

In this paper, we have shown that the method of maximum likelihood can be efficiently used for the derivation of physical approximations of unphysical maps (both non-CP linear maps as well as nonlinear quantum-mechanical transformations). We have applied this method for approximating qubit transformations (the universal-NOT gate, the nonlinear polarization rotation and the map $\rho \longrightarrow \rho^2$). We have analyzed the resulting operations and provided a tool to detect the quality (physical consistency) of the input data. The analysis was performed on selected examples. A more complete analyzes, suggesting a definite tool to distinguish unphysical data will be presented in a separate paper [17].

We have assumed here that the input states of test particles are prepared perfectly, i.e. the action of the initial-state preparator is totally known. Certainly, this is an approximation of a real situation, when test states are prepared with finite precision. This additional source of uncertainty has to be taken into account in realistic estimation procedures of quantum channels.

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