

Comment on “Maximum likelihood reconstruction of completely positive maps”

Jaromír Fiurášek, Zdeněk Hradil, and Miroslav Ježek

Department of Optics, Palacký University, 17. listopadu 50, 772 07 Olomouc, Czech Republic

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The treatment proposed by Sacchi [Phys. Rev. A **63**, 054104 (2001)] does not represent correct solution, because the necessary conditions on trace-preserving completely positive maps are not guaranteed.

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Maximum-likelihood (Max-Lik) principle finds wide variety of applications in quantum theory due to its ability to incorporate necessary conditions as constraints. Max-Lik has been devised for reconstruction of a generic quantum state keeping the positive semidefiniteness in Ref. [1]. Remarkably, it is not only an estimation, but a genuine generalized measurement [2]. In his recent papers Sacchi [3, 4] applied Max-Lik to the reconstruction of completely positive (CP) maps using the numerical algorithm of downhill-simplex method [5]. However, the proposed treatment does not represent the correct Max-Lik solution consistent with quantum theory.

A trace preserving CP map is a linear map from operators in Hilbert space \mathcal{H} to operators in \mathcal{K} . The mathematical formulation of CP map is expressed by the relations (2-4) of the paper [3]. In particular, we can write

$$\varrho_{\text{out}} = \text{Tr}_{\mathcal{H}} [S \varrho_{\text{in}}^{\text{T}} \otimes \mathbf{1}_{\mathcal{K}}], \quad (1)$$

hence the CP map is represented by a positive-semidefinite operator $S \geq 0$ acting on $\mathcal{H} \otimes \mathcal{K}$. The necessary conditions allowing physical interpretation are given by relations (5-7) of Sacchi's paper [3]. This may be treated as a condition analogous to normalization of a density matrix $\text{Tr}[\varrho] = 1$ in quantum state reconstruction. However, in the case of CP map such a condition is given by the relation (6) of [3]

$$\text{Tr}_{\mathcal{K}}[S] = \mathbf{1}_{\mathcal{H}}, \quad (2)$$

where $\mathbf{1}_{\mathcal{H}}$ is an identity. The condition (2) effectively represents N^2 real constraints, $N = \dim \mathcal{H}$. They all are correctly taken into account using the Lagrange multipliers μ_{ij} and introducing the effective log-likelihood functional

$$\mathcal{L}_{\text{eff}}[S] = \mathcal{L}[S] - \text{Tr}_{\mathcal{H}}[\mu(\text{Tr}_{\mathcal{K}}[S])]. \quad (3)$$

Here $\mu = \sum_{ij} \mu_{ij} |i\rangle\langle j|$ and $\mathcal{L}[S]$ denotes the log-likelihood given for example by the relation (1) of the paper [3]. Unfortunately, the problem of finding the maximum of $\mathcal{L}_{\text{eff}}[S]$ under the constraints $S \geq 0$ and $\text{Tr}_{\mathcal{K}}[S] = \mathbf{1}_{\mathcal{H}}$ has not been solved. Using an excuse that “multipliers cannot be easily inferred” the maximization has been done under “looser constraint” $\text{Tr}[S] = N$ only. In this way, Sacchi has fixed the matrix of Lagrange multipliers as $\mu = (K/N)\mathbf{1}_{\mathcal{H}}$, $K = \dim \mathcal{K}$. He was probably inspired by the numerical Max-Lik solution for quantum state estimation [5], where the positive semidefiniteness

and trace normalization represent the only constraints of quantum theory. However, this analogy is misleading and improper in the case of trace-preserving CP maps allowing also nonphysical solutions. Effectively, only a single condition instead of N^2 conditions is imposed in this case. As a consequence the reconstruction does not meet necessary conditions, namely the relation $\text{Tr}_{\mathcal{K}}[S] = \mathbf{1}_{\mathcal{H}}$. This is obvious from the numerical results presented by Sacchi [3], which, in fact, may serve as a counterexample. The necessary conditions $S_p(1, 1) + S_p(3, 3) = 1$ and $S_p(2, 2) + S_p(4, 4) = 1$ are reproduced by the Table 1 as 0.995163231 and 1.006669754. In spite of the author's claim that “the estimated values compare very well with the theoretical ones” the result does not correspond to any trace-preserving CP map. For example, the former relation means that the input state $|0\rangle$ is by such a “device” transformed into a state, where the total probability to appear on the output at the states $|0\rangle$ and $|1\rangle$ is only 0.995. The probability is therefore not conserved. Hence the condition (2) is as important as the positive semidefiniteness itself.

Frankly, the proposed method hardly exhibits any significant advantage in comparison to recently used linear reconstruction methods. Linear approach is feasible for any dimension and all the necessary conditions are also fulfilled “approximately.” Linear treatment corresponds to the maximization of the likelihood (1) in [3] without constraint $S \geq 0$. “Max-Lik” reconstruction of Sacchi [3] imposes positive semidefiniteness and a single constraint. This can be hardly considered as a significant difference since N^2 constraints (2) must be taken into account in full quantum treatment.

Max-Lik reconstruction of trace-preserving CP maps can be formulated correctly [6]. The analogy between quantum state and CP map reconstructions is established on more sophisticated level than assumed in Refs. [3, 4]. As shown in Ref. [6] solution for multipliers and CP map may be obtained using an iterative algorithm. The solution may be found even using numerical downhill simplex method, provided that the effective number of $N^2(K^2 - 1)$ real parameters is used. Making use of the constraint (2), we can express N^2 elements of the matrix S in terms of remaining $N^2(K^2 - 1)$ ones, thus achieving minimal parametrization. The search for the maximum of $\mathcal{L}[S]$ is then performed in $N^2(K^2 - 1)$ dimensional parametric space. At each point, where $\mathcal{L}[S]$ is calculated, we must check whether $S \geq 0$. If this does not hold then we sim-

ply set $\mathcal{L}[S] \rightarrow -\infty$ thereby restricting numerical search to the subspace of physically allowed operators S .

Although the downhill simplex algorithm may be feasible, at least for small dimensions, the necessity to check the positive semidefiniteness of S would slow down the numerical search. This is avoided if one instead utilizes the extremal equations whose solution yields the Max-Lik estimate of CP map [6]. It should be noted here that the formalism employed by Sacchi is very convenient and useful for this purpose. Making use of his notation, we may reformulate the extremal equations for estimated CP map S in a particularly simple and transparent form. We may also straightforwardly extend the results obtained in Ref. [6] to the cases when the input and output Hilbert spaces have different dimensions.

Let ϱ_m denote the various input states that are used for determination of the quantum process. A set of measurements described by positive operator-valued measures (POVM) Π_{lm} is carried out on each corresponding output state. Let f_{lm} denote the frequency of detection of the POVM element Π_{lm} . The estimated operator S should maximize the log-likelihood functional [3, 6]

$$\mathcal{L}_{\text{eff}}[S] = \sum_{l,m} f_{lm} \ln (\text{Tr} [S \varrho_m^{\text{T}} \otimes \Pi_{lm}]) - \text{Tr}[S\lambda], \quad (4)$$

where $\lambda = \mu \otimes \mathbb{1}_{\mathcal{K}}$ is operatorial Lagrange multiplier. We can expand the operator S in terms of its eigenvalues $r_i \geq 0$ and eigenvectors $|\varphi_i\rangle$, $S = \sum_i r_i |\varphi_i\rangle\langle\varphi_i|$. The extremal equations for S can be obtained on inserting this expansion into Eq. (4) and varying with respect to $\langle\varphi_i|$, which leads to

$$S = \lambda^{-1} R S, \quad (5)$$

where

$$R = \sum_{l,m} \frac{f_{lm}}{p_{lm}} \varrho_m^{\text{T}} \otimes \Pi_{lm} \quad (6)$$

and $p_{lm} = \text{Tr}[S \varrho_m^{\text{T}} \otimes \Pi_{lm}]$. Further we have from Eq. (5) that $S = S R \lambda^{-1}$. When we insert this expression in the right-hand side of Eq. (5), we finally arrive at

$$S = \lambda^{-1} R S R \lambda^{-1}. \quad (7)$$

The operator μ must be determined from the constraint (2). On tracing Eq. (7) over \mathcal{K} , we obtain quadratic equation for μ , which may be solved as

$$\mu = (\text{Tr}_{\mathcal{K}}[R S R])^{1/2}. \quad (8)$$

We fix the square root by postulating that μ is positive definite Hermitian operator. The system of coupled Eqs. (7) and (8) may be conveniently solved numerically by means of repeated iterations, starting from some ‘‘unbiased’’ CP map, e.g. $S_0 = \mathbb{1}_{\mathcal{H} \otimes \mathcal{K}}/K$. Note that the Eq. (7) preserves the positive semidefiniteness of S and also the constraint $\text{Tr}_{\mathcal{K}}[S] = \mathbb{1}_{\mathcal{H}}$ is satisfied at each iteration step.

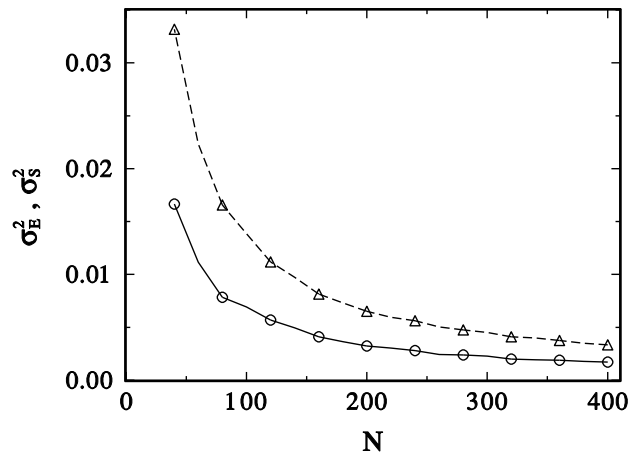


FIG. 1: Variances σ_E^2 (\circ) and σ_S^2 (Δ) for various numbers of measurements N .

In order to explicitly compare the exact Max-Lik estimation with Sacchi’s approximate treatment, we have carried out extensive numerical simulations. Most calculations were based on solution of extremal Eqs. (7) and (8), [Sacchi’s method is then equivalent to assuming that the Lagrange multiplier μ is proportional to identity operator]. Quantitative comparison of the two approaches was based on the variances of estimates S_E (exact) and S_S (Sacchi),

$$\begin{aligned} \sigma_E^2 &= \langle \text{Tr}[(S_E - S_{\text{true}})^2] \rangle_{\text{ens}}, \\ \sigma_S^2 &= \langle \text{Tr}[(S_S - S_{\text{true}})^2] \rangle_{\text{ens}}, \end{aligned} \quad (9)$$

where $\langle \rangle_{\text{ens}}$ denotes averaging over ensemble of all possible experimental data and S_{true} denotes the true CP map. For a given fixed CP map, input states, and output measurements, we have repeated 1000 times a simulation of the measurements and reconstruction of the CP-maps S_E and S_S . Subsequently we have calculated variances (9) as statistical averages over the acquired ensemble.

It should be noted here that Sacchi’s choice of the random input states and random measurements on the output states [3] is not very convenient from the practical point of view. For instance, in case of 10000 measurements, one would have to store a list of 10000 different input states and corresponding 10000 different POVM elements and a mere evaluation of the likelihood functional would require summation of 10000 terms. It is much more practical to use only a moderate amount of different input states and to repeat each measurement on several copies of each state and that scenario was considered in our numerical simulations.

We have found that the exact Max-Lik estimation yields in all cases much lower variance than Sacchi’s approach. This is a direct consequence of the fact that the exact treatment takes into account all constraints imposed on the estimated operator S .

A typical example is shown in Fig. 1. In this case, the quantum process is a unitary transformation of a single

qubit. Six different input states are considered: eigenstates of three Pauli matrices σ_x , σ_y , and σ_z . $3N$ copies of each input state are used. On each corresponding output state, a spin projection along axes x , y and z is measured N times. As can be seen in Fig. 1, the variance σ_E^2 is approximately twice smaller than variance σ_S^2 , which is a significant difference. In fact, for CP-maps which do not represent unitary transformations, such as Pauli damping channel, the difference may be even stronger.

We have also implemented the downhill simplex al-

gorithm and verified that it yields the same results as solution of extremal equations. This confirms that the observed difference between Sacchi's method and exact treatment is genuine and not an artifact stemming from some particular numerical method. Our results show that the exact treatment provides important practical advantage over Sacchi's approximate method, because it significantly reduces statistical error of the estimated CP-map, a fact of central importance for the experiment.

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