Quantum measurement and estimation

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Abstract: Information about quantum systems is inferred from a sequence of measurements made on it. The maximum likelihood (ML) estimation gives an arguably natural optimum approach in quantum theory. The feasibility is shown on valuable examples including quantum phase or entangled spin states.

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In many applications of quantum theory there is a need to determine the quantum state of the system. For this purpose the quantum tomography has been developed. There is an extended bibliography concerning this topic covering various fields of possible applications [1]. However, all the varied and precise experiments which have been carried out over many years and which rely on quantum physics have not used the total amount of information coded in quantum state. This fact is reflected in the standard treatment of quantum tomography. When the standard quantum tomography is adopted for reconstruction of the state from realistic noisy data, one often runs into unphysical results. Standard methods are known to be prone to creation of various artifacts in the reconstructed state. All these flaws are usually paid little or no attention in the scientific literature. They are simply being regarded as unavoidable errors of reconstructions, which fall within the corresponding "error bars". Here we would like to stress that the mentioned drawbacks of the standard tomographic techniques are actually much more serious, especially if the reconstructed state is to be of further use. This seems to be crucial for the potential application in quantum information.

Assume that we are given a finite number N of identical samples of the system, each in the same but unknown quantum state described by the density operator ρ. Given those systems our task is to identify the unknown *true* state ρ from the results of measurements performed on them as accurately as possible. For simplicity we will assume sharp measurements in the sense of von Neumann. Let us assume, for concreteness, that M different outcomes of measurements $\{|y_j\rangle\langle y_j|\}$, $j = 1, \ldots, M$, have been observed. Their relative frequencies f_j then comprise the data form which the true state ρ should be inferred. For the sake of simplicity, the performed measurements will be assumed complete $H \equiv \sum_j \{|y_j\rangle\langle y_j|\} = 1$. This condition will be released later on. The probabilities of occurrences of various outcomes are generated by the true quantum state ρ according to the quantum rule $p_j = \langle y_j|\rho|y_j\rangle$. Notice that due to the presence of noise the standard linear relation $p_j(\rho) = f_j$ has generally no solution on the space of semi-positive definite hermitian operators describing physical states.

Probabilistic interpretation of quantum theory suggests that a sort of statistical treatment of the observed data might be more natural and appropriate. The philosophy of the reconstruction method differs from the philosophy of standard methods. The basic question of the standard methods: "What quantum state is determined by the measured data?" is replaced with a more modest one: "What quantum state is most likely in view of the measured data?" [2]. For this purpose the likelihood functional may be formulated $\mathcal{L}(\rho) = \prod_j \langle y_j|\rho|y_j\rangle^{f_j}$. ML estimation then searches for the state(s) which provide its maximum. Equivalently, one may also consider the log-likelihood known as the relative entropy or Kullback-Leibler divergence $d[\mathbf{f}, \mathbf{p}] = -\sum_j f_j \ln p_j$. As will be seen, the whole process of measurement completed by subsequent ML estimation might be looked at as a single generalized measurement. Thus the ML principle establishes the preferred way of doing the quantum state reconstruction [3].

Extremal point of the likelihood may be reached using several ways. Numerical dowhill simplex algorithm has been used for the cases with low dimension [4], whereas for the two–step iterative algorithm [5] this restriction is not crutial. Moreover, the latter case can be easily interpreted in the formalism of quantum theory. In the first step let as assume that the probabilities p_j of getting outcomes y_j are given by the following linear and positive relation $p_j = \sum_i r_i h_{ij}, \quad \mathbf{p}, \mathbf{r}, \mathbf{h} > \mathbf{0}$. Here $\mathbf{r}$ is the vector describing the "state" of the system. This problem has classical analogy, for example, the reconstruction of blurred image in data processing. The solution of linear and positive (LinPos) problems can be found using the Expectation-Maximization (EM) algorithm. In the case of the discrete one-dimensional problem the unknown object $\mathbf{r}$ is reconstructed by means of the following iterative algorithm:

$$r_i^{(n)} = r_i^{(n-1)} \sum_j \frac{h_{ij} f_j}{p_j(\mathbf{r}^{(n-1)})}, \tag{1}$$

which is initialized with a positive vector $\mathbf{r}$ ($r_i > 0 \, \forall i$). The reconstruction of generic density matrix becomes a LinPos problem provided that eigenbasis diagonalizing the the density matrix is known $\rho = \sum_k r_k |\phi_k\rangle\langle\phi_k|$, $\rho|\phi_k\rangle = r_k|\phi_k\rangle$. Here r_i are eigenvalues of ρ, the only parameters which remain to be determined from the performed measurement. However, the eigenbasis is in general not known and should be estimated as well in the second step. This is achieved using the "rotation" of the basis $\{|\phi_i\rangle\}$ in the "right" direction using the unitary transformation $|\phi_k'\rangle\langle\phi_k'| = U|\phi_k\rangle\langle\phi_k|U^\dagger$. Its infinitesimal form reads $U \equiv e^{i\epsilon G} \approx 1 + i\epsilon G$. Here G is a Hermitian generator of the unitary transformation and ϵ is a positive real number which is small enough.

Consider now the total change of log likelihood caused by the change of diagonal elements of density matrix and rotation of basis. Keeping the normalization condition $Tr\rho = 1$, the first order contribution to the variation reads

$$\delta \ln \mathcal{L}(\rho') = \sum_k \delta r_k (\langle\phi_k|R|\phi_k\rangle - 1) + i\epsilon \, \mathrm{Tr}\{G[\rho, R]\}. \tag{2}$$

The operator R appearing here plays an important role in this treatment. It is semi-positively definite Hermitian operator comprising results of the measurement

$$R = \sum_j \frac{f_j}{p_j} |y_j\rangle\langle y_j|. \tag{3}$$

This operator depends on the old density matrix ρ. Inspection of Eq. (2) reveals a simple strategy how to make the likelihood of the new state ρ' as high as possible. In the first step the first term on the right hand side of Eq. (2) is maximized by estimating the eigenvalues of the density matrix keeping its eigenvectors $|\phi_k\rangle$ constant. The iterative algorithm (1) described above can straightforwardly be applied to this LinPos problem. In the second step the likelihood can further be increased by making the second term on the right hand side of Eq. (2) positive. This is accomplished by a suitable choice of the generator of the unitary transformation. Remembering the norm induced by the scalar product defined on the space of operators , $(A, B) = \mathrm{Tr}\{A^\dagger B\}$, the generator G may be chosen as

$$G = i[\rho, R]. \tag{4}$$

The above described procedure establishes the method how to maximize the likelihood functional starting from some positive initial density matrix ρ. In the course of iterations the Expectation-Maximization step followed by Unitary transformation yield the EMU algoritm [5]. It monotonically increases the likelihood of the current estimate resembling of climbing a hill. In this way the extremal equation for the density matrix [2, 6]

$$R\rho_e = \rho_e \tag{5}$$

is solved. It is a remarkable fact that such a "parameter estimation" of quantum state may be interpreted as a generalized measurement since $R = 1$ on the space where the reconstruction has been achieved.

These results should be modified in the case of incomplete detection. Provided that $H \neq 1$, the closure relation may be always recovered in the form

$$\sum_j H^{-1/2}\{|y_j\rangle\langle y_j|\}H^{-1/2} \equiv 1. \tag{6}$$

This corresponds to the renormalization of the probabilities $p_j = \langle y_j|\rho|y_j\rangle$ in the likelihood to the normalized probabilities $p_j \to p_j / \sum_i p_i$ incorporating the case of incomplete detection. The extremal equation possesses again the form of equation (5) for the renormalized quantities

$$R \to R' = (H')^{-1/2} R (H')^{-1/2}, \quad \rho_e \to \rho_e' = (H')^{1/2} \rho_e (H')^{1/2}, \qquad H' = \frac{1}{\sum_j p_j} \sum_j \{|y_j\rangle\langle y_j|\}. \tag{7}$$

All the conclusions derived for complete measurements can be extended to the case of incomplete measurement as well. This formulation coincides with the estimation accounting for the Poissonian detection statistics. Assume that n_i samples the mean number of particles np_i, where p_i is as before the prediction of quantum theory for detection on the i-th channel and n is unknown mean number of particles. The relevant part of log-likelihood corresponding to the Poissonian statistics reads

$$\ln \mathcal{L} \propto \sum_i n_i \ln(np_i) - n \sum_i p_i. \tag{8}$$

The extremal equation for n may be easily formulated as the condition $n = \sum_i n_i / \sum_i p_i$. Inserting this estimate of unknown mean number of Poissonian particles into the log-likelihood reproduces the renormalized likelihood function.

The generic scheme for indirect observation, namely a quantum measurement followed by estimation, may be demonstrated on several examples. They all can be considered as (quantum) tomography where the signal (quantum state) is inferred from the measured data. The operational quantum phase concepts can be considered as the simplest example of this treatment. The Noh-Fougerés-Mandel phase [7] can be recovered assuming detection of classical phase sensitive signal with Gaussian statistics [8] in interferometry. In this case the “quantum” state is a point inside the unite circle characterized by the phase and visibility. The use of an iterative algorithm is not necessary here since an explicit solution can be found. Moreover, the prediction of phase uncertainty may be significantly improved for detection with coherent states provided that assumption of Poissonian statistics is used [8]. ML phase estimation has been applied also to ideal phase concepts and estimation of other parameters [9].

Due to the structure of the corresponding Hilbert space the identification of an entangled spin state is a more advanced problem. As shown in the paper [5] the data of a realistic experiment [10] can be evaluated using the EMU algorithm. The effect of the noisy measurement can be analyzed. The detailed analysis of various sources of noise clearly demonstrates, that the full ML estimation is superior to other methods.

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